

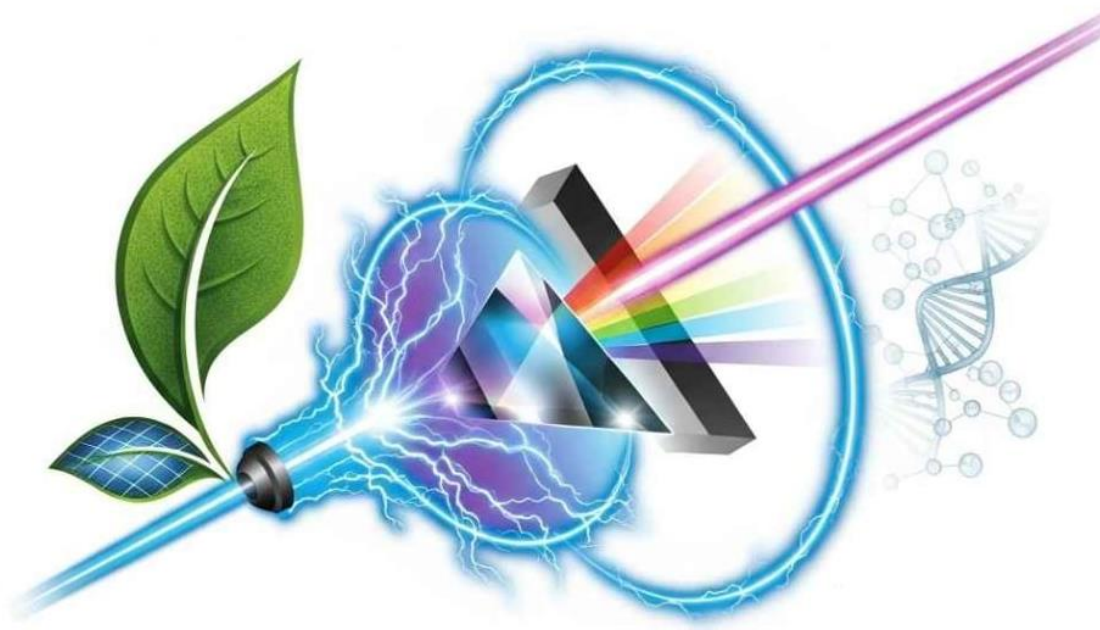
Georgian Technical University – University of Bordeaux

International Workshop:

**“Physics and Technology of Laser-Induced Plasma
for Green Energy and Biomedical Applications”**

Tbilisi, 2-4 October, 2025

Japan – Georgia – Europe



Laser Plasma Applications



**Publishing House
Technical University**

**GEORGIAN TECHNICAL UNIVERSITY
UNIVERSITY OF BORDEAUX**

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Book of Proceedings

Laser Plasma Applications



Tbilisi

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Foreword

It is with great pleasure that we present this volume of proceedings from the International Workshop “*Physics and Technology of Laser-Induced Plasma for Green Energy and Biomedical Applications*,” held in Tbilisi, Georgia, from October 2–4, 2025.

This workshop, hosted by the Georgian Technical University with the support of the International Science and Technology Center (ISTC) and the European Union COST Program Project “Proton-Boron Nuclear Fusion,” brought together a distinguished group of scientists, researchers, and innovators from Japan, Europe, the United States, and beyond. Their shared goal: to explore and advance the frontiers of laser-induced plasma technologies for sustainable energy and next-generation biomedical applications.

The successful organization of this event was greatly facilitated by the valuable partnership and expertise of the University of Bordeaux, notably its renowned research and innovation center in Laser Physics and Technology, as well as by the essential support of the Japanese team of the ISTC and the EU COST initiative “Proton-Boron Nuclear Fusion.” This international collaboration was instrumental in fostering the high-level scientific dialogue that defined the workshop.

The contributions compiled herein reflect the vibrant and interdisciplinary exchange that characterized the event. Over six thematic sessions, participants delved into cutting-edge topics such as laser-driven fusion, proton-boron reactions, nanostructured material synthesis, laser spectroscopy for pathogen detection, and the development of quantum materials for energy and computing. The workshop emphasized not only scientific innovation but also the importance of international cooperation in tackling some of humanity’s most pressing challenges—clean energy transition and accessible, advanced healthcare.

We were particularly inspired by the participation of early-career researchers and students, whose engagement underscores the future of this dynamic field. The call from educators and senior scientists to nurture young talent was both timely and necessary, ensuring continuity and creativity in the years to come.

This workshop marked the beginning of a planned series of collaborative meetings aimed at strengthening ties between Japanese, Georgian, European, and American research communities. The synergy demonstrated here gives us confidence that through shared knowledge and joint projects, meaningful progress in green energy and biomedical technologies is within reach.

We extend our sincere gratitude to all authors, speakers, session chairs, and participants for their valuable contributions. Special thanks go to the organizing institutions and sponsors—with particular

acknowledgment to the University of Bordeaux, the Japanese team of the ISTC, and the EU COST Project “Proton-Boron Nuclear Fusion”—and to the dedicated local team whose efforts made this event possible.

It is our hope that this collection of papers will serve as a useful reference and a source of inspiration for researchers, engineers, and policymakers working toward a sustainable and healthy future.

The Editors

December 2025

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Future of Laser Induced Fusion

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Keywords: Nuclear fusion, Inertial confinement, Direct drive

Abstract

This paper presents an overview of the principles of inertial confinement fusion (ICF) and of recent results, describing what are the difficulties which had to be overcome in order to get ignition, as demonstrated at the National Ignition Facility in the United States in 2022. It also describes the scientific and technological challenges that should be met to be able to develop laser-driven fusion reactors in the next years.

Introduction

The voyage of nuclear fusion started about 80 years ago and it is related to names of famous scientists: A. Sacharov in the Soviet Union and E. Teller in the United States. Indeed, in their respective countries, these are also the fathers of the Hydrogen bomb which indeed is based on nuclear fusion, unlike the atomic bombs based on nuclear fission, as those used in Hiroshima and Nagasaki.

After developing the hydrogen bomb, these scientists thought that it could be possible to use nuclear fusion to develop a source of energy for mankind. This has marked the beginning of research on plasma physics for controlled thermonuclear fusion. In 80 years, research on nuclear fusion has made tremendous progress but indeed it has also provided many disillusiones. The goal of realizing controlled fusion in the laboratory has proven much more difficult than initially estimated.

60 years ago, the laser was invented, opening the field of “Inertial Fusion”. This is related to names like Basov, in the Soviet Union [1], co-Nobel prize for the invention of the laser, and Nuckolls [2], in the United States. The inertial fusion approach has proven to be as difficult as the alternative approach based on magnetic confinement.

Today for the first time in history, we have the demonstration of ignition, the scientific feasibility of fusion, which concludes the first part of this voyage. Indeed, in December 2022, experiments performed on the National Ignition Facility (NIF) of Lawrence Livermore National Laboratory (LLNL) in the U.S. have demonstrated a net energy gain from an inertial confinement fusion (ICF) experiment. By focusing 2.05 MJ of laser energy on a small target containing the thermonuclear fuel (a mixture of deuterium and tritium), they have obtained 3.15 MJ of energy released by the nuclear fusion reactions [3]. This corresponds to a gain $G = E_F/E_L = 3.15/2.05 = 1.54$.

This is an historical breakthrough that validates the principle of Inertial Confinement Fusion and open the pathways to the future possibility of developing fusion reactions for the production of energy. Indeed, the result obtained at NIF has received much interest from the whole scientific community, the media and the public opinion, the decision makers, creating a very favorable attention around nuclear fusion in general [4].

After ignition, NIF reached new milestones in fusion energy, with recent experiments yielding 5.2 and 8.6 megajoules (April 2025) with a net gain >4 , showing a steady progress. It is clear however that in order to achieve ambitious objective of realizing fusion reactors, still many scientific and technological challenges must be met.

The principles of Inertial Confinement Fusion (ICF)

Thermonuclear Fusion studies (both inertial and magnetic) are at the moment based on the nuclear fusion reaction between the heavy isotopes of hydrogen, deuterium and tritium which releases a neutron and an α -particle (i.e. a ^4He nucleus)



In order to win the electric repulsion between the positively charged D and T , these particles must have a very high velocities. The corresponding plasma temperature is at least:

$$T_{min} \approx 5 - 10 \text{ keV}. \quad (2)$$

At the same time, we need to have many fusion reactions to allow for energy gain, i.e. large number of particles and/or a long confinement time. This is expressed by the well-known Lawson's criterium according to which:

$$n_e \tau > 1.5 \cdot 10^{14} \text{ s/cm}^3 \quad (3)$$

where n_e is the plasma electron density (which is equal to the ion density since we deal with hydrogen isotopes) and τ is the confinement time.

Here the two main approaches to controlled thermonuclear fusion differentiates in creating the conditions for fusion. Magnetic Confinement uses low plasma densities and long times (τ of the order of seconds to minutes). Instead ICF is based on achieving very high densities (compression at least 1000 times solid density) and very short confinement times ($\approx$ nsec).

In other words, in the inertial confinement approach we create a hot compressed plasma where the energy is released in a very short time scale by the nuclear fusion reactions thereby creating a sort of micro fusion explosion. In this sense inertial fusion has some analogies, at much smaller energy scales, with the functioning of a hydrogen bomb where the thermonuclear fuel is heated and compressed thanks to the energy released by a primary system (an “usual” atomic weapon based on fission).

This analogy tells us that, in order to avoid an uncontrolled explosion, we can only use a very small quantity of deuterium and tritium. The relation between the energy E_F released by fusion reactions and the mass of the fuel M_{DT} is given by:

$$E_F = N_F \varepsilon_{DT} = \frac{M_{DT}}{2m_i} \phi \varepsilon_{DT} \quad (4)$$

where $\varepsilon_{DT} = 17.6$ MeV is the energy released by one fusion reaction, N_F is the number of fusion reactions, m_i is the average ion mass, and ϕ is the fraction of burned fuel (this is valid for a fuel composed by 50% T and 50% D). In practical units:

$$E_F(MJ) = 3.5 \cdot 10^5 \phi M_{DT}(g) \quad (5)$$

For $M_{DT} = 1$ mg and assuming $\phi = 100\%$, we get $E_F = 350$ MJ. This is equivalent to the explosion of 73 kg of TNT! It is therefore clear that we cannot allow using fuel masses which are larger than a few milligrams!

With such small mass, it is possible to show that the Lawson principle can be satisfied only if we strongly compress the fuel (indeed to densities at least 1000 times the solid density). This is achieved by imploding the fuel thanks to the action of intense laser beams. There are however two different ways of doing so, respectively called direct and indirect laser-drive.

In direct laser-drive (Fig. 1), the laser beams are directly focused on the target: a small spherical shell containing deuterium and tritium. The action of the intense laser light produces a very rapid ionization of matter on the surface of the target, its vaporization, and the creation of a hot plasma rapidly expanding outward. By conservation of momentum (the third principle of dynamics: Newton’s action

and reaction law) the material which has not been evaporated is rapidly pushed inward creating the implosion.

In indirect drive (Fig. 2), the laser beams are focused on the inner walls of a centimeter-size cavity of high-Z material (gold, uranium, ...). A hot plasma is created on the surface and emits soft X-ray radiation which quickly resembles to a blackbody distribution therefore being highly uniform and isotropic. In indirect drive, it is such soft X-ray radiation which produced the ablation of the target and its implosion.

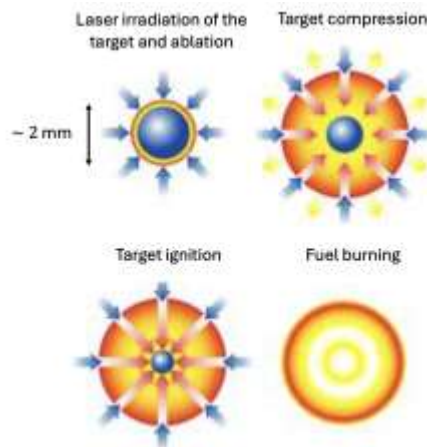


Figure 1. Phases of implosion and ignition of a pellet

Of course, when comparing the two approaches, direct drive has higher efficiency, but more problems with uniformity (since it is difficult to obtain a perfectly uniform irradiation using laser beams). Indirect drive shows better uniformity, due to the intrinsic properties of blackbody radiation but a reduction of efficiency due to the intermediate step of conversion of laser energy into soft X-rays.

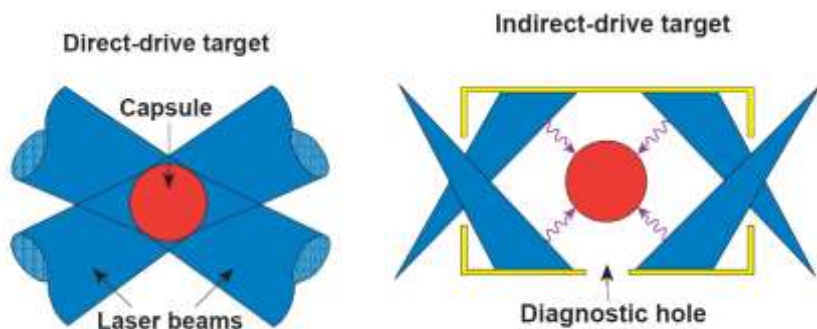


Figure 2. Schemes of direct vs. indirect laser-drive

The typical composition of an ICF target is shown in Fig. 3. The external layer is the so called “ablator” (plastics, SiO₂, Be, Synthetic Diamond). This is the material which is removed (ablated) from the laser pulse and transformed in plasma state rapid expanding outwards.

The second layer (“Fuel”) is a deuterium tritium cryogenic ice with density $\rho = 0.25 \text{ g/cm}^3$ (the density of solid H being 0.25 g/cm^3). Inside this shell there is a DT gas.

The external radius of the target is of the order of $\approx \text{mm}$ and the DT mass of $\approx \text{mg}$. The mass of DT contained in the central region in a gas form is much smaller of the order of $\approx 3 \cdot 10^{-5} \text{ g}$.

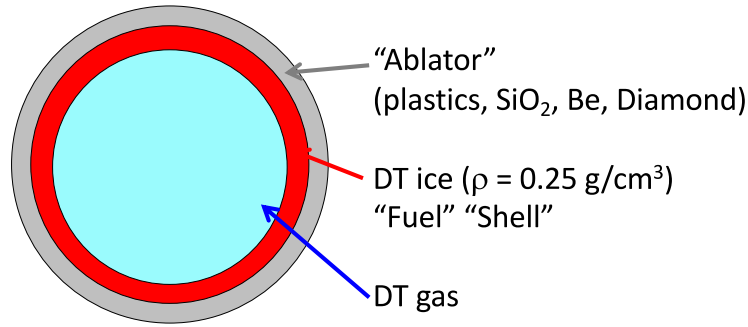


Figure 3. Typical composition of an ICF target

The shell volume is given by $4\pi R^2 \Delta R$, hence a mass of $M = 1 \text{ mg}$ corresponds to a thickness of the DT ice of the order of

$$\Delta R = \frac{M}{4\pi R^2 \rho} \approx 300 \text{ } \mu\text{m} \quad (6)$$

which implies an “aspect ratio” of the target:

$$A = \frac{R}{2\Delta R} \approx \frac{1000}{300} \approx 3 \quad (7)$$

In Inertial Fusion, the ignition point (or «breakeven») takes place when the energy released by the fusion reactions equals the energy delivered by the driver (laser).

To reach ignition we need:

- Compress the fuel at $\approx 1000 \text{ g/cm}^3$, i.e. 4000 times the density of solid DT ice
- Heat the central part of the target at temperatures of $> 5 - 10 \text{ keV}$

The current approach to reach ignition is referred as central hot spot ignition. To understand its meaning let's consider that 1 mg of DT contains a number of ions $N_{\text{DT}} \approx 2 \cdot 10^{20}$ and an equal number of electrons. Heating all these particles to a temperature $T > 5 \text{ keV}$ implies that the thermal energy in the fuel is $E = 2\left(\frac{3}{2} T\right) > 1 \text{ MJ}$. Even if today, we have lasers like NIF able to provide more than 1 MJ , in

reality only a small fraction of the laser energy (typically at most $\approx 10\%$) is coupled to the fuel. All the rest is “lost” in creating the ablated expanding plasma which drives the implosion.

The conclusion is that today the so-called “volume ignition” is NOT achievable!

The principle of central hot spot ignition for inertial confinement relies instead on the creation of a “nuclear burn wave”. This means that we try to heat (and compress) the central gas in the target in order to reach the conditions for satisfying Lawson criterium here and then triggering nuclear fusion reactions which produce α -particles and neutrons. Due to their very low collisionality, neutrons will escape (and actually these are at the end our tool to recover the energy from fusion reactions). On the contrary the penetration range of α -particles in dense matter is very short so they will deposit their energy in a thin layer of the fuel shell surrounding the hot-spot. The temperature in this region will therefore increase so that more fuel reaches conditions for nuclear fusion and more α -particles are created. The cycle repeats and we finally have the propagation nuclear burn wave starting from the hot spot, which gradually involves most of the fuel. The situation is somewhat similar to when we try to set fire to a pile of wood with a match, or when we ignite the gasoline in a combustion engine using a spark.

The advantage of the central spot ignition approach is that we need a lot less energy from the driver because we spend energy to compress all the fuel, but we heat only a very small portion of it (i.e. the central hot spot).

There are two important aspects of the central spot ignition approach. First this approach is clearly dominated by α -particle energy deposition, so we can correctly speak about a “self-heating regime”.

Second, the hot spot is formed by the compression of the DT gas initially contained within the shell. As the pressure in the central spot increases, the imploding shell gradually slows down, and when the pressure of the gas equals the external pressure, the shell stops. We say that the target has reached the “stagnation” and at this point the pressure of the fuel equals the pressure in the hot spot, so we speak about “isobaric fuel assembly”.

The equality of pressures allows to evaluate the conditions in the targets. Since at stagnation, we want that the density in the shell is $\rho_{shell} \approx 1000 \text{ g/cm}^3$ and the temperature in the hot spot is $T_{hs} \approx 10 \text{ keV}$, we can estimate that we will have $\rho_{hs} \approx 100 \text{ g/cm}^3$ and $T_{shell} \approx 1 \text{ keV}$ (this is the order of magnitude obtained by detailed hydrodynamic simulations too). Fig. 4 shows the temperature and density profile at stagnation for a NIF-like target imploded using 1 MJ of laser energy.

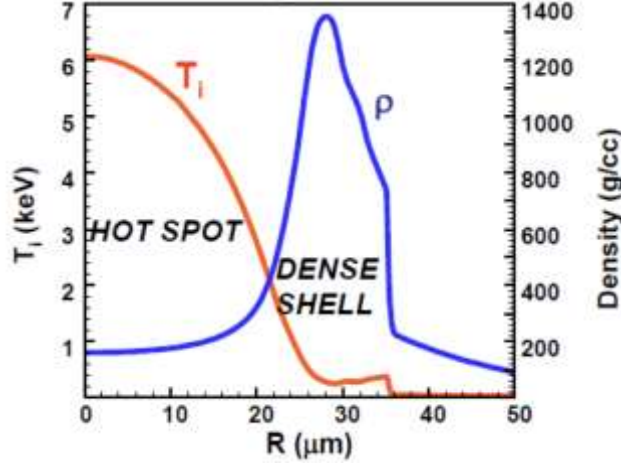


Figure 4. Results of hydrodynamic simulations for a NIF-like target irradiated by 1 MJ laser energy. Temperature and density profile at stagnation (courtesy Riccardo Betti)

In this case, if we assume a hot spot radius $R_{hs} \approx 40 \mu\text{m}$, we can calculate that indeed $M_{hs} \approx 3 \cdot 10^{-5} \text{ g}$, and then the thermal energy contained in the hot spot is $E_{hs} \approx 30 \text{ kJ}$. Such thermal energy is originated by the kinetic energy of imploding shell. At stagnation, part of this energy is converted in compression energy of the fuel and part into thermal energy of the hot spot.

It is then clear that the central hot spot ignition scheme requires very high implosion velocities.

We can also easily calculate the electron and ion density in the hot spot ($n_e = n_i \approx 3 \cdot 10^{25} \text{ cm}^{-3}$) and in the fuel ($n_e = n_i \approx 3 \cdot 10^{26} \text{ cm}^{-3}$). Taking into account that the hot spot due to its very high temperature can be considered a perfect gas, we can then get the final pressure reached at stagnation which is $P \approx 500 \text{ Gbar}$ (in practical units $P(\text{Bar}) \approx 2 \cdot 10^{-18} n_{tot} (\text{cm}^{-3}) T_e (\text{eV})$).

Due to the isobaric conditions, this is also the pressure in the shell fuel (however the dense fuel is not a perfect gas but, due to its very high density, is rather a partially degenerate Fermi gas).

We can notice that the ablation pressure produced by the laser (ablation pressure) is of the order of at most $\approx 50 \text{ Mbar}$. The increase in pressure from this value to the value at stagnation (amplification of a factor $\times 10000$) is largely due to convergence, i.e. to the spherical geometry. It turns out that spherical geometry is essential for inertial confinement fusion, at least within the present state-of-the-art.

Let's also notice that if thermal energy contained in the hot spot is $E_{hs} \approx 30 \text{ kJ}$, by assuming that about 50% of the kinetic energy of the imploding shell goes into heating the hot spot and 50% in compressing the fuel, and if only 10% of the laser energy is coupled to the target (the rest going in the creation of the expanding plasma corona), we see that we need $E_{laser} \geq 1 \text{ MJ}$.

Also, if the mass of fuel is 1 mg, in order to achieve $E_{hs} \approx 30$ kJ, we need an implosion velocity $V \approx 400$ km/s = 400 $\mu\text{m/ns}$. This is the maximum implosion velocity during the free flight phase of the implosion, which is preceded by an initial acceleration phase and a final deceleration phase before stagnation. Hence, we can assume that the average velocity is rather of the order of 200 $\mu\text{m/ns}$. This implies a duration of the implosion of the order of $\tau \approx R/V \approx 10$ ns if $R \approx 2$ mm (this is indeed the typical duration of the laser pulses on NIF).

The laser irradiation intensity on target is therefore $I_L \approx E_{\text{laser}}/(4\pi R^2 \tau) \approx 3 \cdot 10^{14}$ W/cm².

Another important point is that in inertial confinement fusion experiment we need to realize a compression which is as adiabatic as possible. If we compress too fast, we heat the fuel, and a heated material is much more difficult to be compressed. Therefore, in order to reach $\rho_{\text{shell}} \approx 1000$ g/cm³ we must realize a “gentle” quasi-adiabatic compression.

This is obtained by using a laser irradiation which has a special temporal profile composed by 3 parts. Initially we irradiate the target with a rather low laser intensity (the “foot” of the laser pulse). This foot starts the process of laser ablation, creates a shock wave travelling in the shell, produces a first compression (by a factor $\approx 3 - 4$) of the fuel. After that we increase the laser intensity gradually in time (“ramp”). Finally, the laser intensity remains constant in time (“plateau”).

In particular, if the initial shock produced by the foot is too strong it can produce an unwanted preheat in the fuel. Similar preheating effects can be due to the presence of hot electrons or hard X-rays produced by the interaction of the laser beam with the plasma corona.

In order to take these effects into account, we introduce an adiabat-parameter α which is the ratio of the pressure achieved in the compression to the pressure of a perfect adiabatic compression (i.e. for perfect adiabatic compression $\alpha = 1$)

The final problem in ICF implosion experiments concerns target stability. Getting a high implosion velocity guarantees a sufficient shell kinetic energy before stagnation. However, in order to reach such high implosion velocity, we need to use a small mass, i.e. a “thin” shell, i.e. a target with a quite high aspect ratio A . Unfortunately, such thin shells are very sensitive to deformations and can break during implosion, thereby stopping the process. Such deformations are originating from the non-uniformities of laser irradiation: where the intensity is bigger the ablation pressure is bigger, the shell is pushed inward more strongly and distorts during the implosion which is no longer perfectly spherical. But indeed, the situation is even worse because the deformation can be amplified due to a hydrodynamic instability known as “Rayleigh-Taylor Instability”.

This is a well-known instability which develops every time we are trying to accelerate (or keep in place against an acceleration) a dense fluid using a less dense fluid. The classical example is the fact that water falls from a glass when we reverse the glass. This is not due to weight of water because the force applied by air pressure is indeed larger than the gravity force on the mass of water contained in the glass (indeed air pressure can sustain a column of water as high as 10.3 m). This is instead due to perturbations naturally arising at the separation surface between water and air, and to their amplification due to Rayleigh Taylor instability (see fig. 5)

The surface modulations, with initial amplitude Z_0 are amplified in time following an exponential law:

$$Z(x, t) = Z_0 \cos(kx) e^{\gamma t} \quad (8)$$

where $k = 2\pi/\lambda$, λ being the wavelength of the surface perturbation, and γ is the classical growth rate of the instability:

$$\gamma = \sqrt{Akg} \quad A = \frac{\rho_1 - \rho_2}{\rho_1 + \rho_2} \quad (9)$$

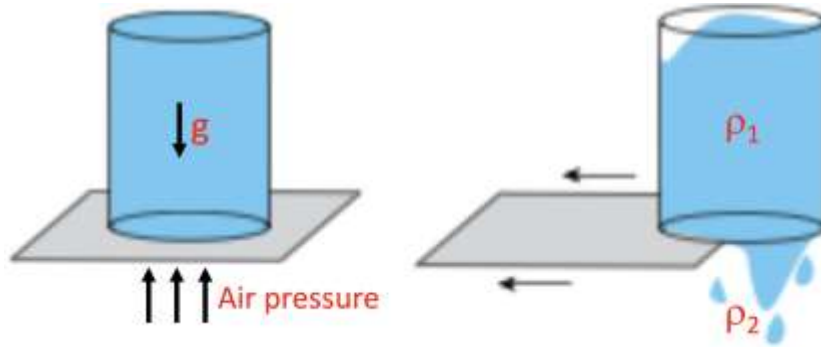


Figure 5. Principle of Rayleigh Taylor instability: Left) the water-air interface is stabilized by a thin paper foil and air pressure sustains the column of water against gravity, right) without the paper foil the perturbations at the interface grow and water finally falls.

Here g is the gravity acceleration and A is the Atwood number. Let's notice that if $\rho_1 > \rho_2$ (water on air) the growth rate γ is real and the perturbation grows exponentially in time. Instead, if $\rho_1 < \rho_2$ (air on water), γ becomes imaginary and the perturbations become a simple wave moving on the surface with constant amplitude and finally possibly damped by friction. Hence the case $\rho_1 < \rho_2$ is hydrodynamically stable.

In laser-plasmas, luckily the Rayleigh Taylor instability is partially stabilized which is expressed by the so called Takabe's formula for the growth rate [5]

$$\gamma = \sqrt{\frac{Akg}{1+kL}} - \beta k V_a \quad (10)$$

where L is the typical scalelength of the plasma in the so-called conduction region (i.e. the region beyond the critical density, where the laser beam cannot propagate), V_a is the ablation velocity (the velocity at which the solid-state matter is eroded), and $\beta \approx 3$ is a constant.

The stabilization effect arises first because instead of a sharp interface, as in the classical Rayleigh Taylor instability, we may have a smoother density profile (as expressed by L) and because the region where the instability begins to develop is “transported away” by ablation (as expressed by V_a).

In any case, even if partially stabilized, the Rayleigh Taylor instability remains one of the major obstacles on the way to performing good implosions, and this is particularly true within the direct-drive approach to ICF.

The quest for ignition on NIF

The National Ignition Facility was completed in the year 2009 and in the same year, NIF started the “National Ignition Campaign” (NIC, 2009-12) which had the goal of demonstrating ignition and indeed to reach a gain $G = E_F/E_L = 20$ [6], which with NIF operating at 1.5 MJ means that $E_F = 30$ MJ. Let’s notice that $G = 1$ implies $N_{neutron} \approx 5 \cdot 10^{17}$ but they only got $\approx 10^{15}$, or just 1 - 2 kJ released from nuclear fusion reactions [7].

NIC experiments were designed using the best hydrodynamics radiative codes available. Despite having been validated in previous years with the results of experiments conducted at much smaller laser energies (on the laser Nova, the antecedent of NIF at Livermore) these codes had several problems:

- The data on equation of state and opacities of materials at high pressures used in hydrodynamics simulations were incomplete.
- The impact of parametric instabilities was underestimated (in particular concerning parametric instabilities in the gas which was put inside the holhraum to limit the expansion of the plasma from holhraum walls and hence the filling of the cavity with plasma).
- And more importantly, the impact of Rayleigh Taylor instability was greatly underestimated.

The Rayleigh Taylor instability arose because of defects in the irradiation uniformity, in the target surface, but also, from the way the pellet was put in position inside the holhraum using a very thin membrane.

Experimentally, the measured convergence ratio was lower than what could be predicted using the value of implosion velocity extracted from experiment. This was a strong indication that the shell was breaking before end of the implosion.

The fact that NIC failed in achieving ignition (although we learned a lot from these campaigns) clearly shows that the goal of achieving ignition is still a scientific challenge rather than a technological challenge. As such it is somewhat “unpredictable”, and this is true for Magnetic Confinement Fusion too.

After the end of NIC, implosion experiments continued on NIF, and at this point the researchers could investigate somewhat different approaches to ignition. In 2013 and 2014, they obtained a first positive result: the energy released from fusion reaction moved up to 7 kJ and finally 26 kJ, against ≈ 2 kJ obtained during NIC. But there was one result which is even more important than the absolute value of released energy. This is the fact that for the first time the contribution from the self-heating induced by α -particles became important. Indeed, considering the implosion performances, it is possible to calculate the final temperature and density value in the assembled fuel, and from this calculate the expected number of fusion reactions, but it is also possible to calculate the increase in temperature produced by α -particle self-heating and see what the increase in nuclear fusion yield produced by such self-heating is. Now it resulted that during NIC the contribution from self-heating was absolutely negligible. Instead, for instance in the shot N130927, the yield calculated on the basis of the performance of the implosion was 7.7 kJ, while the self-heating contributed for an additional 6.6 kJ.

This result was obtained mainly by changing the laser pulse temporal shape. Instead of the low-foot implosions used during NIC, they used “high-foot implosions” characterized by an initial higher irradiation intensity [8]. The high foot pulse set the imploding shell on a higher isentrope α because it launches stronger shocks in the “foot” of the pulse. So, from $\alpha \approx 1.2 - 1.3$, they moved to $\alpha \approx 2.5 - 3$. This result might be a surprise because we have stressed the need for quasi-isentropic implosions in inertial confinement experiments.

The explanation lies indeed in a reduced impact of Rayleigh Taylor instability. A larger initial irradiation means that the created plasma is hotter and expands more rapidly. This implies that the ablation velocity V_a is bigger and also that a longer scalelength λ_a is produced, and these are two factors which contribute to stabilizing the growth rate of the hydrodynamic instability. Indeed, this also shows that the main problem towards achieving ignition during NIC was really the impact of hydro instabilities related to non-uniformities in irradiation and in target quality.

After the results of 2013-24, the best NIF implosions used the High-Foot laser pulse shape and in 2020 they obtained more than 150 kJ of fusion energy, which already allowed to speak about a “Gain” in the fuel (the energy released by fusion reactions became bigger than the total energy invested in compression of the fuel and heating of the hot spot). Finally in 2021 they approached breakeven with 1.35 MJ of fusion energy released by using 1.93 MJ of laser energy on target, and in December 2022, experiments have demonstrated a net energy gain from an ICF experiment.

In addition to using higher foot, NIF results were obtained by several other improvements like:

- The use of different ablaters (in particular HDC, synthetic diamond).
- Different gas pressure in the holhraum.
- Reduced holhraum size and bigger pellet (to improve the coupling of radiation to the target).
- Improved radiation uniformity.
- Improved target quality (roughness).

As written before, this is a historical breakthrough. However, let’s notice that while increasing the isentrope parameter α has been “good” to show ignition, it does not allow to scale ignition to high gain. Therefore, one of the next challenges is indeed to reduce α .

Beyond NIF ignition, towards high gain - The Shock Ignition approach

The National Ignition Facility (NIF) demonstrated ignition, the scientific feasibility of nuclear fusion which is an enormous scientific achievement! However, NIF approach is based on INDIRECT DRIVE which does not seem compatible with requirements needed for future fusion reactors. Indeed, indirect drive implies:

- Complicated targets (difficult to produce, hence expensive, difficult to be precisely aligned at high repetition rates)
- Massive targets (lot of high-Z material injected in the chamber at every lase shot)
- And above all: intrinsic low gain due to the intermediate step of energy conversion from laser to X-rays.

In addition, indirect drive poses “political” problems because it is often considered as “proliferating” since it reproduced on a micrometric scale several aspects of the mechanism of operation of a hydrogen bomb (for a discussion on this issue see ref [9]).

For all these reasons, in order to progress towards “inertial fusion for energy”, we need DIRECT DRIVE.

Unfortunately, we know that Direct Drive is prone to the impact of non-uniformities and hydrodynamic instabilities. A possible solution to this problem consists in the separation of the compression phase and the ignition phase in implosion experiments. This is indeed the common approach to so-called “advanced” schemes for ignition: Fast Ignition and Shock Ignition.

Fast ignition has been proposed in 1994 by M. Tabak and co-workers at Livermore [10]. Despite being very interesting from the physical point of view, it is based on exotic and non-scalable physics (laser-plasma interactions in the relativistic regime) and it requires the developments of a laser facility delivering ≥ 100 kJ in 10 ps which is far beyond the state-of-the-art in laser technology. Therefore, we will not further discuss Fast Ignition here. For a recent review on this topic see [11].

On the contrary, Shock Ignition is compatible with present-day laser technology. This scheme has been proposed by R. Betti, J. Perkins et al. at the University of Rochester [12] and somewhat anticipated by V.A. Shcherbakov many years before in the Soviet Union ([13], although this work didn’t find further developments).

Again, the phases of compression and ignition are separated.

- First a thicker and more massive target is imploded using ns laser beams at lower implosion velocity $V \approx 240$ km/s (against 350 – 400 km/s in the classical approach). Since the target is thicker, it is intrinsically more resistant towards the impact of hydro instabilities. However, the low kinetic energy of the imploding shell does not allow to create a central spot which is sufficiently hot to start nuclear fusion reactions.
- Therefore, ignition is achieved by using a final laser spike which irradiates the target at high laser intensity (up to 10^{16} W/cm²) with a duration of several hundred ps. This launches a strong shock (≥ 300 Mbar at the ablation front) which converges spherically at target center providing the conditions for triggering the fusion reactions.

In addition to being compatible with present-day laser technology and being more resistant against hydro instabilities, another advantage of shock ignition is that the final fuel assembly is non isobaric (the assembly would be isobaric at the end of the compression phase but the final shock increases the pressure in the hot spot) which implies higher gains because in a way the hot spot is more effective in producing fusion reactions.

Preliminary experiments on Shock-ignition experiments have been made on the OMEGA laser facility of the University of Rochester. Omega is the only laser facility explicitly studying the direct-drive approach to inertial fusion. Unfortunately, despite being a big laser, it can only deliver about 30 kJ

of laser energy on target, i.e. it is a sub-ignition laser facility which is good to study the physics of direct-drive implosions, but which cannot achieve ignition and gain.

In the experiment described in ref. [14] (see Fig. 6), it was shown that the performance of the implosions was improved when a shock launching power spike was added at the end of the laser pulse. The neutron yield increased but, even more importantly, the “Yield over Clean” (YOC) was observed to improve.

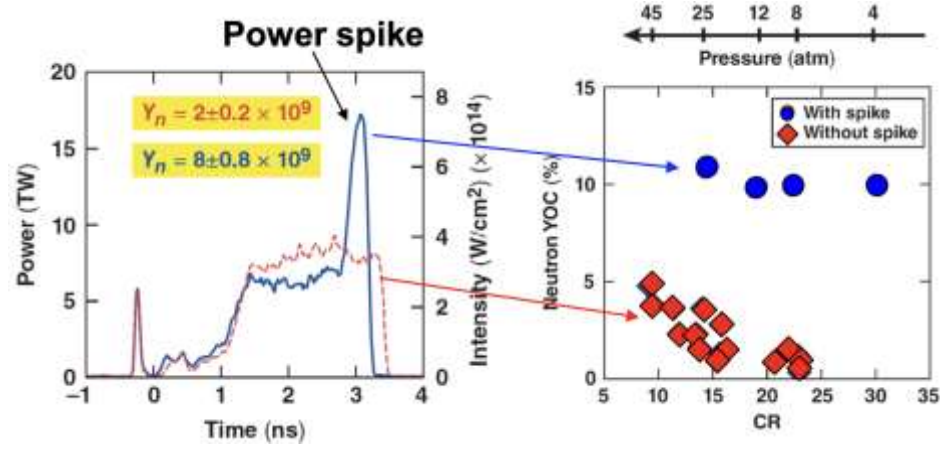


Figure 6. Results from the experiment at the Omega laser facility. Comparison between a normal laser temporal shape and the laser pulse with a final laser spike at the end, (courtesy Wolfgang Theobald)

The YOC is the ratio between the experimentally measured neutron yield and the neutron yield calculated in 1D hydrodynamic simulations. Of course, in current experiments we have $YOC < 1$ (otherwise the problem if ICF would have already been solved!). Fig. 6 b shows that without the final spike, YOC was between 5 and 1 and was decreasing when the convergence ratio increased, showing the difficulty in driving implosions to very small target radii (the convergence being the ratio between the initial pellet radius and the final one). On the contrary, with the final spike, YOC was approaching a value of 10% even for convergence ratios of 30.

Since in 1D hydrodynamics simulations there is of course no place for hydrodynamics instabilities, the YOC directly describes the impact of hydro instabilities on implosion performance. The closer YOC is to 1, the more the implosion is 1D, the smaller the impact of Rayleigh Taylor instability. In this sense, YOC is a better diagnostic for implosion performance than the simple absolute value of neutron yield.

Therefore, the experiment at Omega showed that the laser pulse shape typical of shock ignition can potentially really limit hydro instabilities effects.

Despite these encouraging results, there are many physical unknowns of Shock Ignition which must be studied, understood, and mastered before we can proceed to full-scale demonstration experiments.

The first one is related to laser-plasma parametric instabilities arising at high laser intensities (to $\approx 10^{16}$ W/cm²). These are nonlinear interaction phenomena coupling the laser waves to electron plasma waves or ion-acoustic plasma waves. The coupling of the laser with electron plasma waves gives origin to Stimulated Raman Scattering (SRS) and to Two Plasmin Decay (TPD). The coupling of the laser with ion-acoustic plasma waves gives rise to Stimulated Brillouin Scattering (SBS). These instabilities (SBS and SRS) can reflect part of the incoming laser light, thereby reducing the laser to target coupling. In addition, SRS and TPD can also excite a non-thermal electron distribution, i.e. produce “hot” or “suprathermal” electrons.

In the past 50 years of research on inertial fusion, the regime of high laser intensities has always been deliberately avoided because it is not beneficial for implosion, largely because of these parametric instabilities which are very hard to be controlled. Now high laser intensities become necessary for the shock ignition approach but indeed we know very little about this regime of laser-plasma interaction. How the parametric instabilities develop? How much light do they reflect? This requires specific experimental and theoretical research and the development of advanced numerical simulation codes that take these effects into account.

The topic of hot electrons deserves some specific mention. Usually in ICF hot electrons have always been considered as very dangerous. Due to their long propagation range, they can deeply penetrate the target and preheat the fuel thereby making its compression much more difficult and more expensive in energetic terms (they increase the adiabat of the implosion). In shock ignition however, the hot electrons are produced by the final laser spike practically at the end of the implosion. Hence, they come at late times, when the fuel has already been compressed (the areal mass density of the shell $\rho\Delta R$ is already very large). In these conditions, if hot electrons are not too energetic, they will be unable to penetrate the dense material, so they could indeed be not harmful or even beneficial, increasing laser-target coupling in presence of a very extended plasma corona and contributing to increase the pressure of the final ignition shock [15]. Again, it is very important to study how many hot electrons are generated, at what energy, and what is their effect on target hydrodynamics.

A final important point concerns the possibility of demonstrating shock ignition on existing laser facilities. While today laser technology allows to produce the kind of temporal pulse shape which is needed for shock ignition, the big laser facilities like NIF have been built for indirect laser drive. This

means that the laser beams do not come uniformly distributed around the interaction chamber, i.e. around the target, but are concentrated in two poles corresponding to the two entrance holes of the holhraum. Adapting such installations to direct drive experiments could be possible by using the so-called “Polar Direct Drive” ([16] PDD) which means repointing the laser beams on a sphere for optimal illumination. The drawback is that this implies reducing the available energy because the beams which are coming more tangentially on the target have larger focal spots, so the intensity is reduced. Then in order to maintain the same intensity in all points, the energy of the beams which have not been repointed (and still have a smaller focal spot) should be reduced.

Although preliminary experiments on PDD have already been done, there is no final answers about the possibility of replacing laser-direct drive with PDD.

In conclusion, “on paper” shock ignition is feasible and could bring large advantages, however there are many physics points which needs to be understood and mastered, including parametric instabilities, cross beam emery transfer, hot electrons generation and their impact, the acceptable degree of non-uniformity in the compression and in the ignition phases, the possibility of using Polar Direct drive. All these studies constitute the elements of a Roadmap for shock ignition (see Fig. 7). The development of a full program relies on scientific credibility and addressing the physics issues using existing intermediate-scale facilities like OMEGA in the U.S., PALS, ORION, Vulcan, Phelix in Europe, Gekko in Japan, SG II UP in China, etc. Clearly international collaboration is a key factor here.

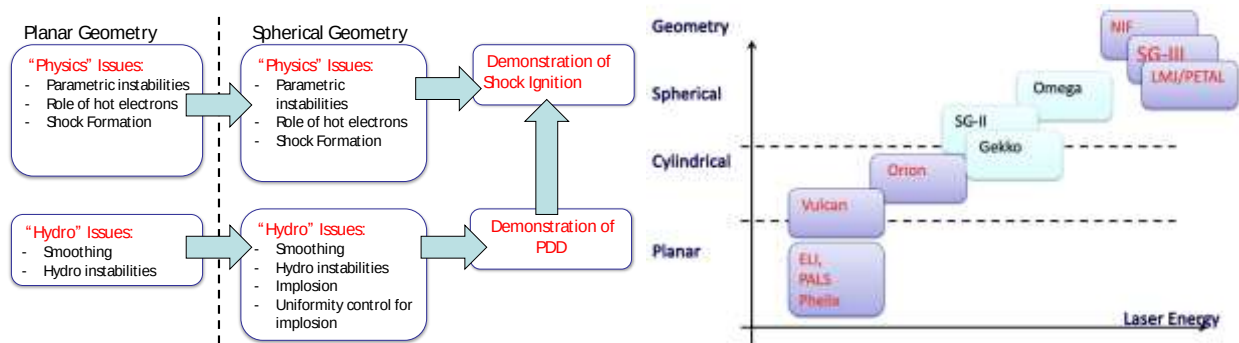


Figure 7. Elements of a roadmap on shock ignition. Left) with respect to the physical issues (for clarity “hydro” issues have been separated), Right) with respect to available intermediate laser facilities. This scheme refers to existing laser facilities (NIF, LMJ, SG III, ...) which are based on indirect-drive illumination. Of course, a laser facility specifically designed for the direct-drive approach wouldn't need to use the PDD illumination of the target.

Perspectives of Inertial Fusion Energy (IFE) Technical and scientific challenges

There are today two big «Megajoule» lasers for inertial fusion. The first one is of course NIF, at Lawrence Livermore National Laboratory, in California, near San Francisco. The second one is Laser Megajoule (LMJ) at the CESTA research center in Le Barp, near Bordeaux in France. LMJ is run by CEA.

The third biggest laser in the world is Shenguang-III (SG III) in Mianyang in China which can deliver an energy above 100 kJ. However, recently China started the realization of a new laser facility which should be bigger than NIF. Although recently a preliminary design for a 10 MJ laser has been published [17], probably this new facility may not reach the 10 MJ energy as speculated in some journal news [18,19].

These are «single shot» machines which can be used to study the physics of inertial fusion, but which are not scalable to a fusion reactor.

The guidelines from the U.S. National Academies of Sciences, Engineering, and Medicine (NASEM) to the U.S. Department of Energy, require the realization of a 50 MW Fusion Plant that produces electricity from fusion at the lowest possible capital cost (“Pilot Plant”). Even such small power plant would need a laser system working at high repetition rate and fusion gains much bigger than the values of ≈ 4 currently obtained in NIF experiments, or even $G = 10$ as initially expected from NIC and now envisaged for the future high gain campaigns on NIF. Future “real” energy production requires that the laser system should work at repetition rate between 1 and 10 Hz, and the fusion gain for each shot is of a few hundred or even 1000.

Gains of ≈ 1000 are theoretically possible. Using the formula for E_F reported at the beginning of this lecture note, and assuming $\phi = 100\%$, we see that we can get $G = 1000$ with a fuel mass of 6 mg and $E_L = 2$ MJ. Using a more realistic value $\phi = 30\%$, it implies a mass of 18 mg [notice that NIF results ($E_F = 3.15$ MJ) mean that $\phi \approx 1\%$ only].

Beyond achieving a high gain, we need to face 3 big challenges related to 1) lasers, 2) targets, and 3) materials.

Challenge 1: Lasers

Today’s laser systems have a very low efficiency, conversion of electrical to laser energy is $< 1\%$. At NIF the energy stored in the capacitor banks was about 384 MJ to produce 2 MJ of laser energy. Also, lasers like NIF, LMJ, SG-III can fire typically 1 shot/day and they use 350 nm light (near UV, 3w of Nd:

glass lasers). This is very good from the point of view of dynamic compression but has the bad drawback of potentially inducing larger damage to optics which in turn will reflect on the lifetime of the facility.

In order to think about a reactor, we need consider the possibility of using 2ω light (532 nm) to reduce damage to optics, develop broadband lasers (because this is a way to reduce parametric instabilities), and develop laser systems which are more efficient ($\geq 10\%$) and can work at high repetition frequency (10 Hz).

Diode pumping of laser systems appears to be promising in increasing both the repetition rate and the efficiency (efficiency up to 20% have already been demonstrated although not yet demonstrated with high energy laser systems).

Challenge 2: Targets

Today's cryogenic target costs ≈ 10000 \$, they require many days of preparation and characterization, and they need $\approx$ hour to be injected in the chamber and properly aligned.

In order to think about a reactor, we need to develop cheap technology ($< 1\$/\text{target}$), develop a capability of mass production of targets, develop techniques for target injection and alignment at ≈ 1 Hz (which implies the design of specific target insertion and tracking systems). Again, all this does not seem possible with indirect drive!

Challenge 3: Materials

The problems here are on one side related to tritium breeding and tritium handling and recycling system and resolving the related security and safety issues.

On the other side, there are the problems of activation of materials which imply the production of some quantity of radioactive wastes but also the structural damage of the materials subjects to intense neutron irradiation, which again reflects on the lifetime of the facility. There is a need of identifying adequate materials for chamber construction and protection and in parallel develop remote handling techniques and possibly develop intense laser-based neutron sources for testing materials in pulsed regime.

Many of these issues are common to Magnetic Confinement Fusion too which means that synergies are possible in this field.

These are difficult challenges that need time in order to be properly addressed. Hence, a realistic timeline to develop a direct- drive reactor is necessarily of the order of 30 years with 3 major steps of about 10 years each including the production of knowledge, the construction of machine, the time needed to produce and analyze results for the technology transfer.

Despite such difficult challenges, there is today a climate of optimism towards the developments of inertial fusion, both within the scientific community, and in the public opinion and decision makers, which is of course the direct consequence of NIF results. For the first time in the U.S., there is a discussion on the possibility of developing national projects on Inertial Fusion Energy (IFE) as a future source of energy while until now, the research at NIF was mainly related to defense (indeed NIF was developed within the “Science Based Stewardship of the Nuclear Stockpile” programme [9]. This has brought to issuing, for instance, the “Basic Research Needs report” [20], a guide for DOE to establish a national IFE program in the USA.

In Europe, Germany, which was traditionally against ICF due to the link to defense research, has suddenly changed its attitude towards IFE and is now the country which is more supportive of IFE in Europe [21]. Everywhere we saw a big shift from defense driven research to energy oriented one.

This was also reflected in the creation of several start-ups related to inertial fusion, in Europe we have Focused Energy [22], Marvel Fusion [23], and GenF [24]. In general, the presence of start-ups and the interest of industries towards IFE, can be a positive factor, accelerating the research progress in the field and creating the industrial base for the development of future reactors based on inertial fusion. However, such start-ups often propose over-optimistic goals, often promising the realization of fusion reactors and the supply of electrical energy from fusion within a 10-years horizon. This is clearly unrealistic seen all the scientific and technological challenges which we listed before. Indeed, such rash statements could have negative consequences in the medium term for the entire fusion sector. As scientists working in the field of fusion, our goal is today to couple a realistic approach to the optimism which is justified because of recent demonstration of ignition.

Indeed, these are the objectives of the HiPER+ initiative [25] and its published roadmap to fusion in Europe [26]. Recently HiPER+ has been endorsed and financed by EUROFUSION with the objective of producing a “conceptual design for a direct-drive implosion facility in Europe [27]. The project is involving 30 research groups from 12 European countries, assembling the vast majority of the scientific community working on Inertial Fusion and physics of laser-produced plasmas in Europe. We propose the design of a facility which will be able to demonstrate ignition and gain using direct-drive and shock ignition, associated to PW kJ beams for diagnostics. The facility will also address the technical issues needed to move towards fusion reactors and commercialization of energy:

- laser architecture and conversion efficiency (including the need of large bandwidth)
- high repetition rate,

- target production and injection...
- study of radiation damage, optics lifetime,
- first wall and mantle issues, tritium breeding, etc.

This unique facility would enhance the level of IFE research in Europe and create conditions for European leadership in associated technologies. The laser energy should be in the range of ≥ 1 MJ engaging industry for developments. Of course, this will be a multibillion-euro project which will need to enter the ESFRI Roadmap.

Conclusions

We are clearly entering a new era in thermonuclear fusion. The recent breakthrough obtained at NIF, the commitment to fusion via large facilities like ITER, NIF, LMJ, make the demonstration of net energy production from fusion possible in a few years. Still, we will need a lot of work to progress towards the development of fusion reactors, and this work is not simply only technological, but it includes major scientific challenges. In the field of inertial fusion, the development of fusion reactors relies on the progress of direct laser drive and the ability of mitigating the growth hydrodynamics instabilities possibly through the shock ignition approach.

Today IFE is a credible approach to Fusion Energy, however the challenges are still very big, both technologically and scientifically. Even with infinite funding, the time needed to address such challenges cannot be indefinitely compressed. Therefor now it is necessary to maintain the scientific enthusiasm and optimism but keep scientific credibility, which is the content of the HiPER+ project.

While we need to define a strategic way forward, it is also clear that the dream of controlled thermonuclear fusion for producing energy for mankind may finally become true.

ACKNOWLEDGEMENTS

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Laser-Synthesized Quantum Materials for Energy and Quantum Information Technologies

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Abstract

Laser-induced plasma synthesis has emerged as a powerful bottom-up approach for the fabrication of quantum materials with precisely engineered electronic, spin, and phononic properties. By exploiting ultrafast, nonequilibrium plasma–matter interactions, this method enables the formation of nanoparticles, nanoclusters, and two-dimensional nanostructures with exceptional purity, controlled defect density, and tunable quantum confinement. This chapter presents a comprehensive review of the physical principles underlying laser–plasma synthesis and demonstrates how this versatile technique supports two strategically important technological domains: green energy conversion and quantum information technologies. Particular emphasis is placed on graphene–silicon heterostructures for photovoltaic applications, laser-synthesized quantum dots for spectral engineering, and ultra-clean spin-based qubit platforms such as nitrogen-vacancy centers in nanodiamonds and silicon quantum dots. By integrating materials physics, quantum coherence considerations, and device-oriented perspectives, the chapter positions laser–plasma synthesis as a unifying platform for next-generation energy and quantum technologies.

Keywords: Laser–plasma synthesis, quantum materials, graphene–silicon heterostructures, quantum dots, nanodiamonds, NV centers, spin qubits, photovoltaics, green energy

1. Introduction

Bottom-up synthesis strategies offer an alternative paradigm, enabling the assembly of functional materials from atomic and molecular precursors under highly controlled conditions. Among these approaches, laser-induced plasma synthesis occupies a unique position [1–5]. The interaction of high-intensity laser radiation with condensed matter produces extreme, transient conditions—characterized by high temperatures, high pressures, and rapid quenching—that are difficult or impossible to achieve using

equilibrium chemical methods. These nonequilibrium environments favor the formation of metastable phases, size-confined nanostructures, and defect configurations that are particularly advantageous for quantum technologies.

This article provides a comprehensive overview of laser–plasma synthesis as an enabling platform for quantum materials. After outlining the fundamental physical mechanisms of the technique, we explore its application to green energy technologies, with a focus on graphene–silicon heterojunction photovoltaics and quantum-dot-based energy conversion concepts. We then examine the role of laser-synthesized materials in quantum information science, emphasizing spin-based qubits and coherence preservation. The chapter concludes with a discussion of current challenges, scalability considerations, and future research directions.

2. Physical Principles of Laser–Plasma Synthesis

2.1 Laser–Matter Interaction and Plasma Formation

Laser–plasma synthesis typically relies on pulsed lasers with power densities exceeding 10^7 – 10^9 W·cm^{−2} [1, 6, 7]. When such radiation is focused onto a solid target, rapid energy deposition leads to localized melting, vaporization, and ionization. Within nanoseconds, a dense plasma plume composed of atoms, ions, electrons, and molecular fragments forms above the target surface. (Fig.1).

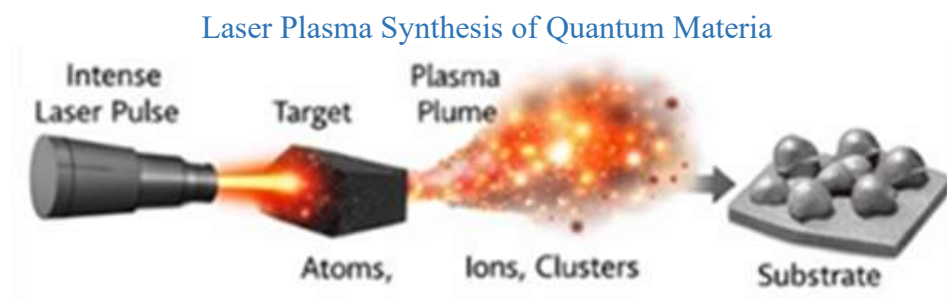


Figure 1. Schematic illustration of laser–plasma synthesis. High-intensity laser irradiation produces a transient plasma plume that undergoes rapid expansion, cooling, and nucleation, leading to the formation of quantum-confined nanoparticles and nanostructures with controlled size, composition, and defect configuration.

The characteristics of this plasma—temperature, ionization degree, expansion velocity—are governed by laser parameters such as wavelength, pulse duration, fluence, and repetition rate. Short-pulse lasers favor nonthermal ablation mechanisms, while longer pulses promote thermal vaporization. In both regimes, the plasma serves as a highly reactive medium for nanoparticle formation.

2.2 Plasma Expansion, Cooling, and Nucleation

Following its formation, the plasma plume expands into the surrounding environment, which may consist of vacuum, inert gases, or chemically active atmospheres [6–8]. Rapid adiabatic expansion leads to cooling on microsecond timescales, driving the system into a supersaturated state. Under these conditions, homogeneous nucleation of nanoclusters occurs, followed by growth through condensation and coagulation. (Fig.2).

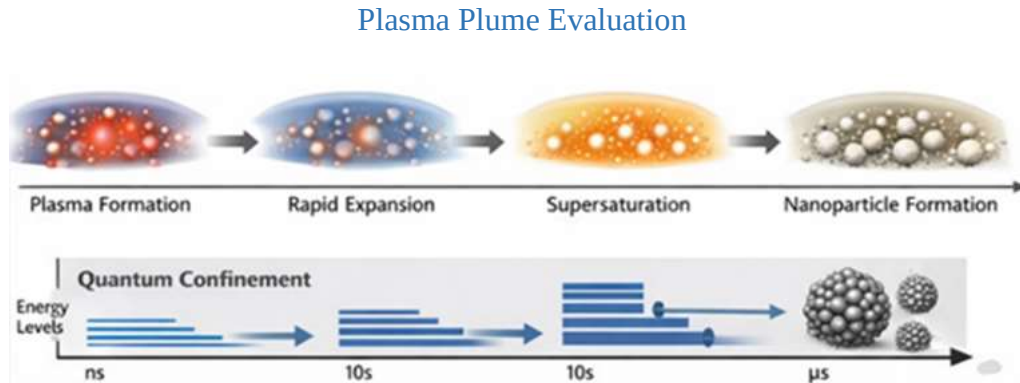


Figure 2. Temporal evolution of the laser-induced plasma plume. Ultrafast cooling and quenching enable stabilization of quantum-confined nanostructures and metastable phases inaccessible under equilibrium conditions.

The ultrafast quenching intrinsic to laser–plasma synthesis effectively freezes nonequilibrium structures, enabling the stabilization of metastable phases and well-defined quantum-confined nanoparticles. This feature is particularly important for materials whose functional properties depend sensitively on size, crystallinity, and defect configuration.

2.3 Control Parameters and Quantum Property Engineering

A key advantage of laser–plasma synthesis lies in its exceptional tunability. Material properties can be engineered through:

- Laser parameters: wavelength, pulse duration, fluence, and repetition rate;
- Ambient conditions: gas composition and pressure, which influence cooling rates and chemical reactions;
- Target composition: single-element, composite, or multilayer targets enabling alloy and heterostructure formation.

Through careful optimization of these parameters, it is possible to produce nanoparticles with diameters ranging from a few nanometers to several tens of nanometers, narrow size distributions, and tailored electronic band structures. Of particular relevance to quantum technologies is the ability to engineer spin-active defects and minimize unwanted impurity incorporation.

3. Laser-Synthesized Quantum Materials for Green Energy

3.1 Graphene–Silicon Heterostructures for Photovoltaics

Silicon remains the dominant material in photovoltaic technology; however, its performance is constrained by recombination losses and limited spectral utilization [9,10]. The integration of graphene with silicon has attracted considerable interest as a pathway toward enhanced device efficiency. Laser–plasma deposition enables the direct synthesis of few-layer graphene nanostructures onto silicon substrates, forming clean, well-adhered heterojunctions [10–13].

In graphene–silicon solar cells, graphene serves not only as a transparent conductive layer but also as an active component in charge separation and transport. Its high carrier mobility and tunable work function facilitate efficient extraction of photogenerated carriers, while its mechanical flexibility and thermal stability improve device robustness. Moreover, the unique phonon spectrum of graphene contributes to reduced carrier–phonon scattering, thereby lowering recombination losses. (Fig.3).

Graphene – Silicon Heterojunction

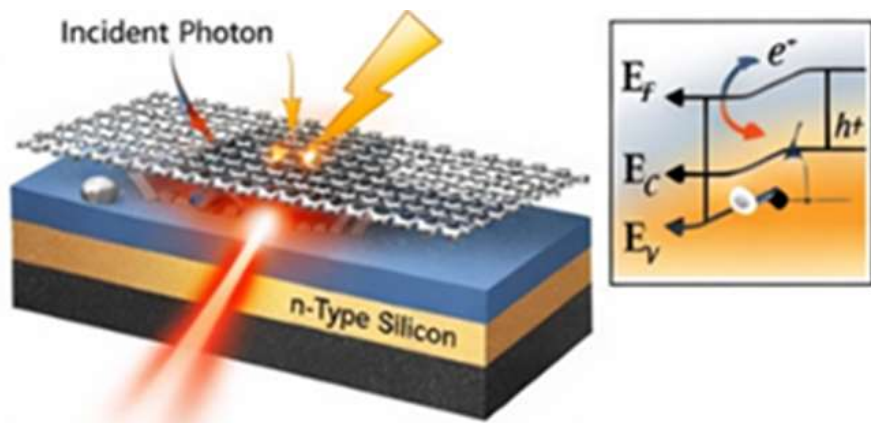


Figure 3. Graphene–silicon heterojunction formed by laser–plasma deposition. Graphene functions as both a transparent conductive layer and an active charge-extraction medium, enhancing carrier separation and reducing recombination losses.

3.2 Quantum Dots and Spectral Engineering

Laser-synthesized semiconductor quantum dots offer precise control over size-dependent bandgaps, enabling spectral tuning for optimized solar energy harvesting [14–17]. Materials such as PbS, CdSe, and silicon quantum dots can be produced with narrow size distributions, allowing absorption to be matched to specific regions of the solar spectrum. When integrated into quantum-dot-sensitized solar cells or tandem architectures, these materials provide pathways toward surpassing conventional efficiency limits. (Fig.4).

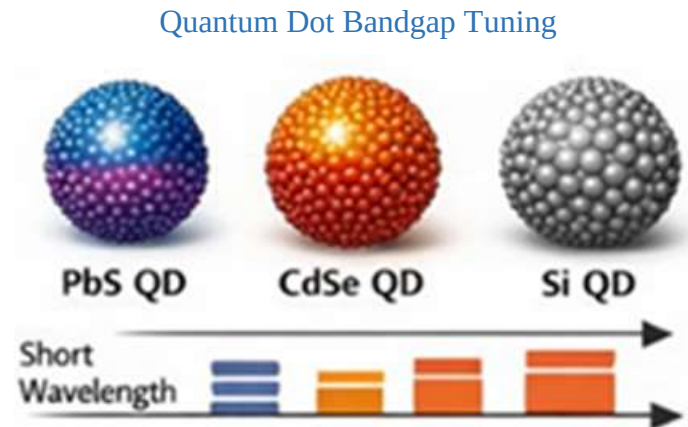


Figure 4. Size-dependent quantum confinement in laser-synthesized semiconductor quantum dots. Precise control of nanoparticle diameter enables tunable bandgaps for spectral engineering in photovoltaic and optoelectronic applications

3.3 Beyond Photovoltaics: Thermoelectrics and Catalysis

Nanostructuring achieved via laser–plasma synthesis is also advantageous for thermoelectric materials, where reduced thermal conductivity and enhanced electronic transport are desired. Additionally, laser-synthesized nanocatalysts with clean surfaces and controlled defect densities show promise for photoelectrochemical energy conversion and hydrogen production.

4. Quantum Information Technologies Enabled by Laser Synthesis

4.1 Nanodiamonds with Nitrogen–Vacancy Centers

Nitrogen–vacancy (NV) centers in diamond represent one of the most mature solid-state qubit platforms, combining long spin coherence times with optical addressability at room temperature [18–

21]. Laser ablation of carbon targets in nitrogen-containing atmospheres enables the one-step synthesis of nanodiamonds incorporating NV centers. The catalyst-free, gas-phase environment minimizes metallic impurities and uncontrolled defects, leading to superior spin coherence properties. (Fig.5).

NV Center in Nanodiamond

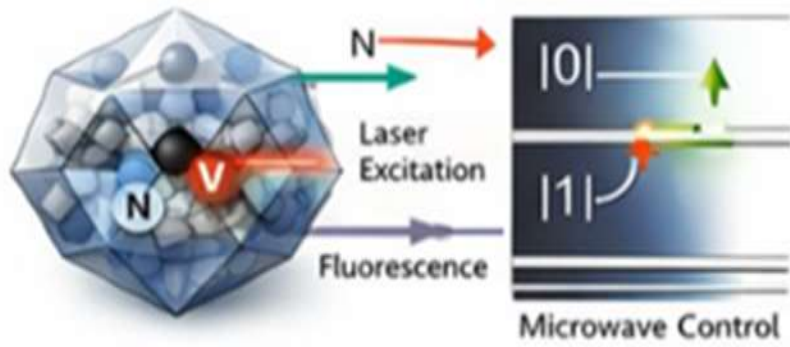


Figure 5. Laser-synthesized nanodiamond hosting a nitrogen–vacancy (NV) center. The ultra-clean synthesis environment minimizes decoherence sources, enabling long spin coherence times suitable for quantum sensing and quantum information processing.

4.2 Silicon Quantum Dots and Spin Qubits

Silicon-based spin qubits benefit from weak spin–orbit coupling and the availability of nuclear-spin-free isotopes [22–25]. Laser pyrolysis techniques allow the production of highly crystalline silicon quantum dots with well-defined confinement energies. These structures can function as isolated qubits or be assembled into scalable arrays compatible with existing semiconductor technologies. (Fig.6).

Silicon Quantum Dot Qubits

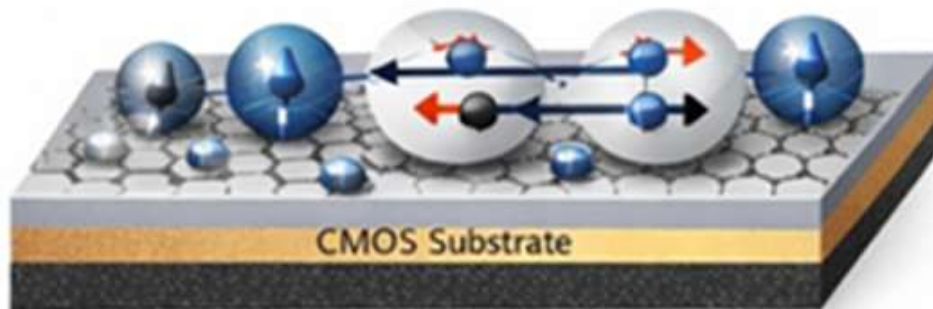


Figure 6. Silicon quantum dots synthesized by laser pyrolysis as spin qubit platforms. Weak spin–orbit coupling and isotope purification support long coherence times and scalability.

4.3 Toward Superconducting and Hybrid Qubits

Although less explored, laser–plasma synthesis also offers routes to producing nanoscale superconducting materials with controlled stoichiometry and defect landscapes. Such materials may support hybrid quantum architectures combining photonic, spin, and superconducting degrees of freedom.

5. Convergence of Energy and Quantum Technologies

A notable feature of laser-synthesized quantum materials is their relevance across traditionally distinct technological domains [33–37]. Concepts such as phonon engineering, spin coherence, and defect control play critical roles in both energy conversion and quantum information processing. Laser–plasma synthesis thus functions as a bridging technology, enabling cross-fertilization between green energy research and quantum science. (Fig.7).

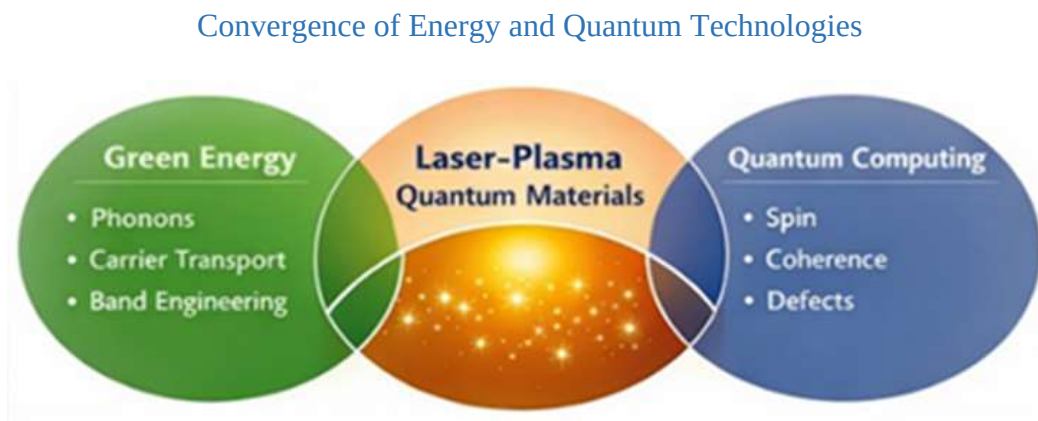


Figure 7. Conceptual convergence of green energy and quantum information technologies enabled by laser–plasma-synthesized quantum materials.

6. Challenges, Scalability, and Industrial Outlook

The rapid evolution of modern technologies in energy conversion, information processing, and sensing increasingly depends on the availability of materials whose properties are governed by quantum mechanical phenomena. Quantum confinement, spin coherence, topological protection, and engineered defect states have become central concepts in contemporary materials science [33–37]. Conventional top-down fabrication routes, while highly developed for microelectronics, often struggle to deliver the level

of atomic-scale purity, structural flexibility, and quantum-state control required for these emerging applications.

Despite its advantages, laser–plasma synthesis faces challenges related to large-scale production, reproducibility, and integration with device fabrication workflows. Advances in high-repetition-rate lasers, continuous-flow reactors, and in situ diagnostics are expected to address many of these issues. For high-value applications such as quantum computing and advanced photovoltaics, the benefits of superior material quality may outweigh cost considerations.

7. Conclusions

Laser–plasma synthesis represents a uniquely powerful and conceptually distinct approach to quantum materials engineering. By operating far from thermodynamic equilibrium, this technique enables direct access to transient plasma states, ultrafast quenching, and defect-controlled growth pathways that are inaccessible through conventional chemical or top-down fabrication methods. As a result, laser-synthesized nanostructures exhibit a combination of purity, structural flexibility, and quantum functionality that is particularly well suited for next-generation technologies.

A central conclusion of this chapter is that laser–plasma synthesis should be viewed not merely as a nanoparticle production technique, but as a platform for quantum property engineering. Through precise control of plasma dynamics, ambient chemistry, and growth kinetics, it becomes possible to design materials in which electronic confinement, spin coherence, phonon transport, and defect states are deliberately tailored at the nanoscale. This capability is essential for both high-efficiency energy conversion systems and scalable quantum information platforms.

In the context of green energy technologies, laser-synthesized graphene–silicon heterostructures and semiconductor quantum dots illustrate how quantum-level control can translate directly into macroscopic performance gains. Reduced recombination losses, enhanced carrier extraction, and phonon engineering demonstrate that quantum materials are no longer a purely academic concept, but an active component of energy-device optimization. Importantly, the same synthesis principles that govern carrier dynamics in photovoltaics also govern decoherence mechanisms in quantum systems.

From the perspective of quantum information science, the ability to fabricate ultra-clean spin-active nanostructures—such as nanodiamonds with nitrogen–vacancy centers and silicon quantum dots—addresses one of the most critical challenges in the field: preservation of quantum coherence in realistic

material environments. Laser–plasma synthesis offers an intrinsic advantage by minimizing unwanted impurities and enabling controlled defect incorporation, thereby supporting longer coherence times and improved qubit reproducibility.

Perhaps most significantly, laser–plasma synthesis emerges as a bridging technology between energy science and quantum engineering. Concepts such as spin–phonon coupling, defect engineering, and nonequilibrium growth dynamics unify these domains and suggest a convergent research pathway. Future developments may include laser-synthesized topological materials, hybrid spin–photon systems, and quantum–energy co-designed architectures.

In summary, laser–plasma synthesis provides not only a route to advanced materials, but also a framework for thinking about quantum functionality as a design variable. As laser technology, in situ diagnostics, and scalable reactor designs continue to advance, this approach is poised to play a central role in the realization of quantum-enabled energy systems and fault-tolerant quantum information technologies.

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Warm Dense Matter Characterized by Laser Shock

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Abstract. Recent advanced technologies of high-power lasers and the related proving methods enable us to characterize the extreme states of shocked materials including warm dense matter. High power pulsed laser generates strong shock waves that achieve high pressure and high temperature state and deform at high strain rates in nanoseconds. The shock compressed state is proved by optical methods to determined pressure, density, and temperature as well as some physical properties. Bright and Ultrashort x-ray pulse (X-ray free electron laser, XFEL) visualizes the shocked state in terms of atomic level structural information. The results can be applied to simulate condensed matter physics and chemistry, natural impact conditions and planetary interiors. I will introduce some recent experimental results together with the related technical methods.

Introduction

Dynamic compressions utilized by shock wave have been known to generate unique extreme conditions in terms of pressure, temperature, density, strain rate, quenching rate, and gravity field in a limited time. Shock compression research fields open up high density science and are applied in various researches dependent upon the shock strength [1]. Recent advanced relation of a material between temperature and pressures over 1000 GPa [2] where materials become warm dense matters (Fig. 1). They differ from plasma in temperature and density. The observation of laser-shocked materials in shock compressed depends upon optical measurements of velocity and thermal emission. Typical optical velocity measurement is provided by the velocity interferometer for any reflector system (VISAR) [4]. Particle velocity measurements are limited at relatively low shock pressures because a reflector is set as

a mirror in the target. Shock velocity, however, is measured at high shock pressures because the shock front becomes a reflector in transparent materials. Thermal emissions from the shocked state and shock front are collected to determine the shock temperature profile as a function of time. In laser-shock experiments, streak cameras are used to record the emission at a fixed narrow band in visible wavelength range, called streaked optical pyrometer (SOP) [5]. VISAR and SOP are two main methods to determine the shocked state.

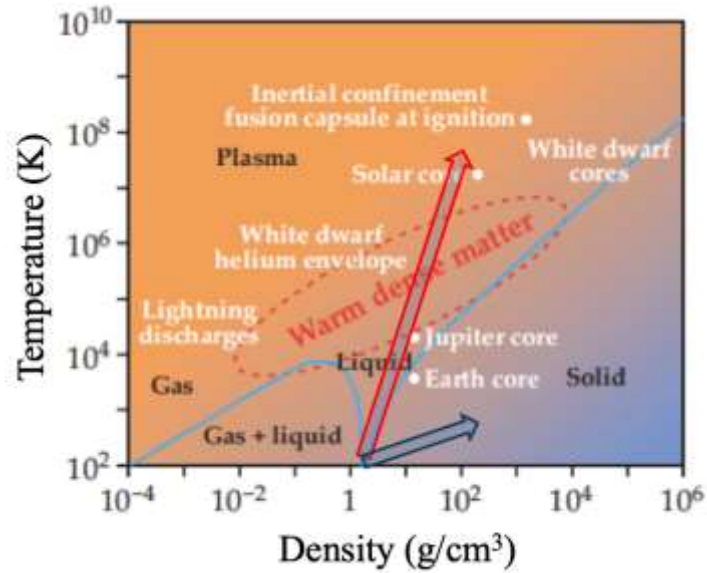


Figure 1. Temperature-density relations among solid, liquid, gas, and plasma compared with star and planetary conditions and inertial confinement fusion modified from [3]. Red and black arrows indicate directions of compression by shock wave and ramp wave, respectively. Note that ramp compression keeps temperature low enough and stays as solid at very high pressures.

Figure 2 shows a dynamic response of a solid during shock compression process at relatively low pressure where an elastic precursor wave and a phase transition are observed. Although an elastic wave is often observed if the Hugoniot elastic limit is high enough in laser shock experiments, a single shock wave will be induced at high pressure conditions induced by laser shocks and VISAR measurements works effectively. Shock compressed state is analyzed by three Rankine-Hugoniot equations [8]. These relations provide the relationships between shock velocity and particle velocity and between pressure and density by measuring two unknown parameters in the equations. The Rankine-Hugoniot equations do not provide temperature and structure information at Hugoniot states. Temperature is calculated thermodynamically from the internal increase by shock compression that is given Fig. 2. Schematic illustration of shock compression and release process. The first wave is elastic and the second plastic

wave of low-pressure phase (LPP) induces a phase transition to generate a high-pressure phase (HPP) as the third wave. When a rarefaction wave catches up the shock wave, release process starts as adiabatic process. The pressure (P) and temperature (T) drop quickly but T remains as the residual temperature from where T drops slowly through thermal conduction. There is a three-wave structure of the shock front.

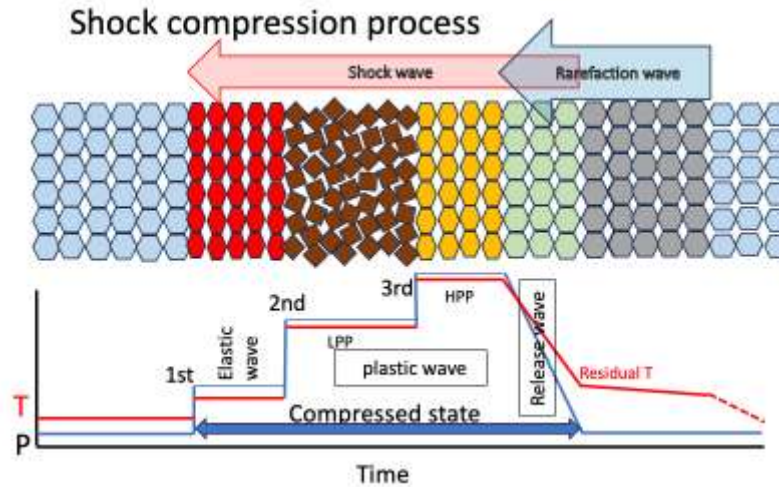


Figure 2. Schematic illustration of shock compression and release process. The first wave is elastic and the second plastic wave of low-pressure phase (LPP) induces a phase transition to generate a high-pressure phase (HPP) as the third wave. When a rarefaction wave catches up the shock wave, release process starts as adiabatic process. The pressure (P) and temperature (T) drop quickly but T remains as the residual temperature from where T drops slowly through thermal conduction. There is a three-wave structure of the shock front.

by the Rankine-Hugoniot equations or determined through the Plank equation from the emission measurements. The structure information at atomic level is visualized by in situ x-ray diffraction using x-ray free electron laser (XFEL) [9].

Some experimental results on planetary materials

(1) SiO₂

SiO₂ displays a series of phase transitions as one of the most popular minerals. Many high pressure studies have been conducted in a wide range of pressures experimentally and theoretically. There are four forms of SiO₂ (fused silica, quartz, coesite, and stishovite) available for laser shock experiments. Figure 3 illustrates the results of the four SiO₂ starting materials.

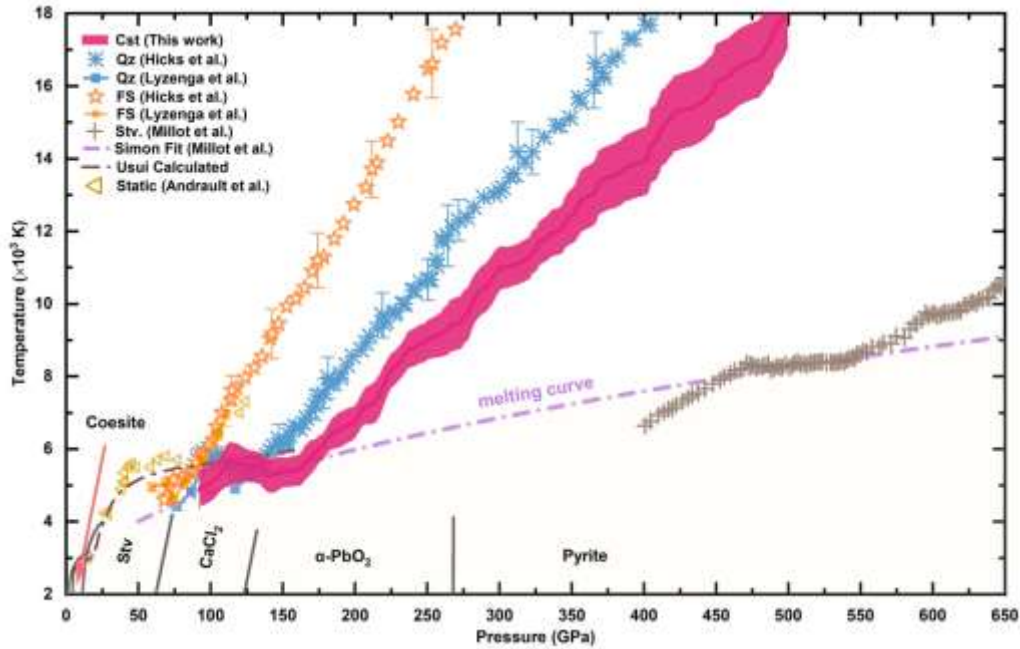


Figure 3. Pressure-temperature diagram illustrating shock compressed SiO_2 compared with the equilibrium phases [12]. FS and Qz are low-pressure phases of fused silica and quartz by Lyzenga et al. [10] and Hicks et al. [11], and Cst and Stv are high-pressure phases of coesite by Feng et al. [12] and stishovite by Millot et al. [13], respectively. The melting curve is from [13].

The initial density is 2.20 g/cm^3 for fused silica, 2.65 g/cm^3 for quartz, 2.92 g/cm^3 for coesite, and 4.29 g/cm^3 for stishovite, and affects the shock compressed path on the pressure-temperature diagram (Fig. 3). The structural changes in SiO_2 have been investigated using XFEL. From fused silica stishovite is crystallized in nano second time scale [14,15] but not through coesite that is expected to crystallize under equilibrium. Shock recovery experiments on quartz indicated a metastable phase crystallization [16] and subsequent XFEL and detailed crystallographic studies [17] have confirmed it to be a rosielite-structured high-pressure phase [18]. The structural changes from coesite by laser-shock compression are known also to depend upon the pressure and time [19]. According to [19], the metastable phase of defect-type NiAs-type (d-NiAs- type) phase appears at pressures of 58-131 GPa, but seifertite ($\alpha\text{-PbO}_2$ -type) appears as the high pressure phase on the release path from 131 GPa. CaCl_2 -type high pressure phase was never observed at Hugoniot and release states. These dynamic processes have been investigated using synchronized XFEL delaying techniques at SACLA [9].

We have investigated typical planetary materials including forsterite (Mg_2SiO_4) [20-22] and calcite (CaCO_3) [23,24] using laser shocks.

(2) Iron

Iron is the major constituent of Earth and planetary cores and has been employed as a tool element to human beings historically. The bcc to hcp phase transition at 13 GPa, the first detected by shock compression techniques [25], made the historic epoch in shock compression science. The Hugoniot has been determined to pressure over 400 GPa [26,27] but does not indicate melting from the shock velocity-particle velocity relation. Hugoniot for heated iron at 1275 K was studied experimentally including Hugoniot for fcc iron [28]. The bcc to hcp transition has been investigated in situ X-ray diffraction techniques [29,30]. Three-wave structure below 35 GPa includes the Hugoniot elastic limit, bcc-hcp transition, and quenched fcc, and expanded bcc after the release [30].

Melting of iron at high pressures has been investigated through measurements of sound velocity [31,32] and shock temperature [33]. The sound velocity and temperature drop at the time of melting and detect onset melting. After complete melting they will increase monotonically with increasing pressure. Both measurements show a consistent melting condition that starts at 225 GPa and completes at 270 GPa. The melting curve is approximated by Simon-Glatzel equation [33]. The onset melting condition of iron have been confirmed by X-ray diffractions [34-36] that indicate that hcp phase is stable before melting at 225 GPa. Figure 4 illustrates the summary of experimental results and theoretical simulations of iron melting.

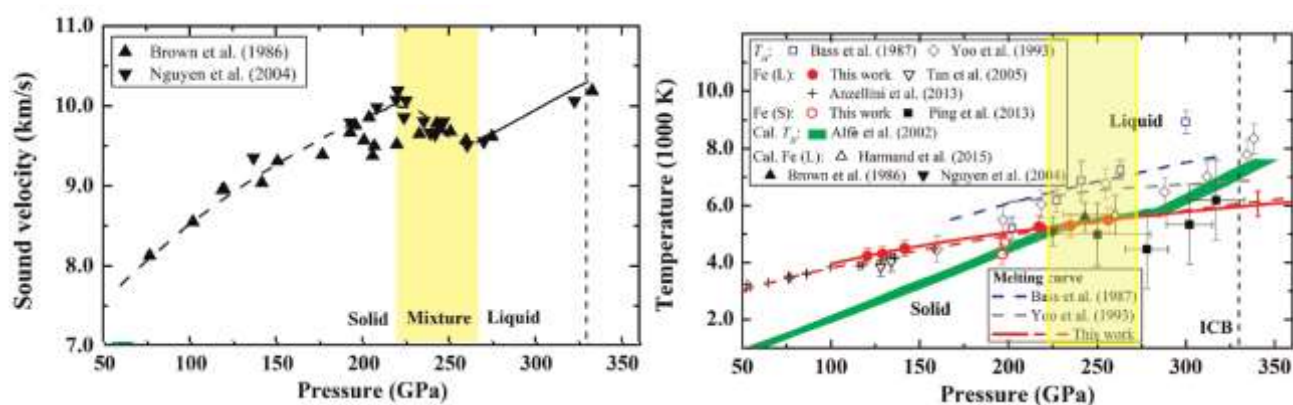


Figure 4. Sound velocity and temperature of iron determined by shock at pressures of 50-350 GPa. Yellow bands indicate the pressure range of melting. Cited from [33]. Note that shock data (red circles) are consistent with the results by the previous shock data [34-39], theoretical simulations [41] and an extension of static data by Anzellini et al. (2013) [39] below 200 GPa.

Summary

This paper reviews shock compression techniques to determine Hugoniot and properties of warm dense matters, especially on typical planetary materials. Recent progress to use high power lasers and XFEL facilities enable us to investigate structural, optical, thermal, and electronic properties as well as density and temperature. These data provide further understanding of materials behaviors under extreme conditions, including planetary interiors and severe impact events, will contribute to modelling the warm dense matters.

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Laser Printing Technologies

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Keywords: Laser printing, two-photon polymerization, biofabrication, 3D brain models

Abstract. This article provides a brief overview of our recent publications on laser printing technologies and their applications. We report on laser printing of nanoparticles, living cells and microorganisms, as well as the development of 3D brain models and laser-assisted microbial culturomics.

Introduction

There is a wide variety of laser printing technologies, most of which are genetically related to laser-induced forward transfer (LIFT) [1,2]. (LIFT) is a direct-write, non-contact, laser-based additive manufacturing/printing technique in which a laser pulse propels material from a donor substrate to a receiver substrate with high spatial precision. It enables deposition of solid, liquid, biological, and functional materials without nozzles, solvents, or masks. A transparent carrier supports a thin donor film (ink, metal, biomaterial). A focused laser pulse is directed through the transparent carrier and absorbed locally at the interface. Rapid localized heating or vaporization launches a micro-jet or the lifted layer(flyer) of material across a micro-gap onto a receiver substrate. Usually in LIFT nanosecond laser pulses are used. Application of picosecond/ or femtosecond laser pulses enables finer feature control and high-resolution laser printing. It has been demonstrated that femtosecond laser printing can be used for controlled fabrication of spherical metal (Au, Ag, Cu, Fe, etc.) and semiconductor (Si, Ge, etc.) with precisely adjustable radii between 100 and 800 nm and their accurate positioning on desired substrates [3–6]. The sizes of the laser-printed nanoparticles can be reduced dramatically by using lithographically structured donor films consisting of islands of material [7]. The printed nanoparticle arrays can be used as sensors and metasurfaces to control light. Resonant excitation of electric and magnetic dipole moments in dielectric nanoparticles can be used for the realization of efficient metasurface mirrors [8]. Applications of laser printed nanoparticles for additive manufacturing, for the generation of

monodisperse colloidal nanoparticle solutions, and for the development of novel materials have been recently discussed in [9].

Laser printing of cells and microorganisms

Laser printing of living cells is one of the fascinating and promising approaches in biofabrication. Laser printing is biologically gentle, when done correctly, and is characterized by very high cell viability > 95%. Unlike nozzle-based extrusion or inkjet printing, laser-assisted methods are nozzle-free, which means: non clogging, no shear stress, no damage for cells, freedom in bioink formulation [10]. This makes it especially attractive for printing of fragile or sensitive cells (like stem cells, induced pluripotent stem cells (iPSCs), neurons, etc.) [11–13]. Also, high cell density corresponding to the cell density in living organs can be printed. With its micron-scale accuracy, laser printing is ideal for printing of microvasculature [14], patterning of vasculature precursors, and investigations of cell-cell and cell-environment interactions [15].

Traditional microbiology techniques often fail to culture many microbial species. Laser printing of microbial cells can provide serious advantages in this field. It can be used for isolation of “unculturable” microorganisms and preparation of pure cultures [16-17]. It can be applied for investigations of cell-cell and cell-environment interactions [18]. Laser printing of cells and microorganisms enables unprecedented control and flexibility in realization and engineering of living systems at microscopic scales. In a recent paper [19], laser printing of microorganisms from clinical oral biofilms into highly organized arrays of microbial colonies, which are suitable for co-culturing and molecular analyses, has been demonstrated. Laser printing offers promising perspectives for generating on-demand biofilms and culture collections for research and clinical use.

3D human brain models

The human brain is the body's complex "command center". It remains a fascinating object and understanding how it works represents a very important scientific challenge. The brain receives and sends electromagnetic signals via nerve cells (neurons), synapses and neurotransmitters. In modern theories of human brain, biological intelligence (BI) and learning occur through the strengthening or weakening of synaptic connections between neurons, a process known as synaptic plasticity. Artificial intelligence (AI)

neural networks mirror this process through the adjustment of “weights” — numerical values that determine the strength of connections between artificial neurons.

Due to extreme complexity of active human and/or animal brains, it is challenging to make predictive experiments with them. During recent years, we see a rapid development of different in vitro 3D brain models (see [20-22] for review). These models represent a paradigm shift and allow to perform much more simple and predictive experiments. Many of these models are based on brain organoids. Brain organoids are simplified, lab-grown models of brain tissue, usually derived from human stem cells or iPSCs. They can mimic certain aspects of early brain development such as cell types, layering, and electrical activity. Recently, a novel concept of Organoid Intelligence (OI) has emerged. OI is aimed at the combination of brain organoids with artificial intelligence systems to generate learning and memory, with the goals of modelling cognition and enabling biological computing applications [23].

In our work [24], we used two-photon polymerization technique for laser fabrication of scaffolds, shown in Fig. 1, for long-term (over 120 days) in vitro development of human iPSC-derived functional neuronal networks. It has been demonstrated that iPSC-derived neuronal progenitors develop into functional neuron–glia networks consisting of different cell types corresponding to their occurrence in the human brain.

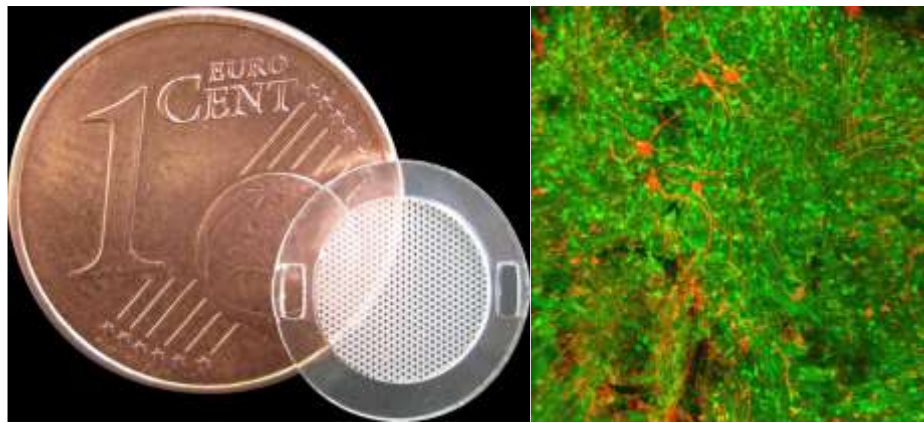


Figure 1. Scaffolds fabricated by two-photon polymerization technique for the development of brain models, commercially available from Laser nanoFab GmbH (left) and functional neurons-glia network developed inside these scaffolds (right).

In the developed brain model one can control the number of different cell types, record action potentials. Computer added training, supported by AI, and stimulation of functioning 3D brain models could allow to understand how BI and complex brain functions (learning, thinking, consciousness) emerge

from 3D network of neurons [25]. Using microelectrode arrays (MEA), special sequences of electrical signals generated with the help of AI can be used for stimulation and training of 3D brain models.

Concluding remarks

In this paper the current state-of-the-art of our work on the development of laser printing technologies is reviewed. Laser printing of nanoparticles and nanoparticle arrays is promising for applications in printed electronics (for fabrication of RF antennas, interconnects, sensors), biomedical devices (biosensors and implant interfaces), photonics and plasmonics (metasurfaces), rapid prototyping of micro and nanodevices. Laser printing of living cells has great potential for tissue engineering and regenerative medicine (due to layer-by-layer tissue assembly and realization of precise tissue architecture). Printing endothelial cells in predefined patterns [14] could allow guiding the formation of microvasculature and blood vessels which is still one of the biggest challenges in tissue engineering and biofabrication. Laser printing is well suited for creating highly reproducible, microscale tissue models for in-vitro disease models and drug testing. The high resolution of laser printing opens up new possibilities for fundamental studies of interactions between cells and between cells and their environment. Laser printing of microbial cells can revolutionize industrial microbiology by given access to many currently unculturable species. Printing of iPSCs and neuronal stem cells for realization of 3D brain models can help us to understand how the human brain, “most complex machine in the universe”, works.

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Proton boron fusion for laser driven medical applications

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Keywords: radioisotope, proton boron fusion, medical applications, ^{43}Sc , ^{44}Sc

Abstract

Using the petawatt, high-repetition-rate VEGA-3 laser at Centro de Láseres Pulsados (Salamanca), we demonstrated laser-driven production of radioisotopes via proton- and α -particle-induced nuclear reactions. Irradiation of boron-rich targets triggered hydrogen–boron fusion, generating intense α bursts that can induce secondary nuclear transmutations. γ -ray spectroscopy with an HPGe detector confirmed the production of ^{43}Sc , ^{44}Sc , ^{48}Sc , ^7Be , ^{11}C , and ^{18}F .

At a repetition rate of 0.14 Hz, we achieved yields of $\sim 4.3 \times 10^3$ nuclei of ^{43}Sc and $\sim 1 \times 10^5$ nuclei of ^{44}Sc per shot using natural calcium. These results highlight the potential of high-intensity lasers for compact, on-demand production of medically relevant radioisotopes for imaging and targeted radionuclide therapy.

Introduction

Radioisotopes play an important role in modern medicine, enabling sensitive diagnostic imaging, targeted radiotherapy, and theranostics. Today, most medical radionuclides are produced in nuclear reactors that are costly, infrastructure-intensive, and geographically limited. Indeed, there are only four research reactors in Europe (accounting for a very large part of radioisotope production in Europe and in some cases also at world-level). They also face aging, strict regulations and limited availability.

Conventional cyclotrons typically deliver low-energy protons, favoring long-living isotopes, while only a few higher-energy facilities, such as ARRONAX [1] and U-120M [2], can reach energies of protons up to 80 MeV and allow for the production of short-living radioisotopes. These machines can also accelerate α -particle beams which allows for the production of different kind of radioisotopes, often with very interesting characteristics. However, due to the cost and the complexity of the machines like

ARRONAX and U-120 M, this technology is not widespread, and they produce only a very limited amount of radioisotopes, indeed just sufficient for pre-clinical studies.

Short-living isotopes such as ^{43}Sc ($T_{1/2} = 3.89$ h) are particularly attractive for PET imaging due to favorable decay properties and reduced radiation dose to healthy tissue. However, their brief half-lives make centralized production impractical, highlighting the need for new approaches. As a result, hospitals often rely on longer-lived isotopes to compensate for transport delays, excluding short-living radionuclides with potentially superior clinical performance.

High-intensity, petawatt-class lasers offer a transformative alternative. They can accelerate protons and α -particles to energies sufficient for nuclear reactions, enabling compact, on-demand radionuclide production without large magnets, nuclear fuel, or reactor infrastructure. Laser systems could operate near hospitals, provide access to short-lived isotopes, and open novel reaction channels, such as α induced production via hydrogen–boron fusion.

There is a strong societal need of increasing radioisotope production to meet increasing demand (Fig. 1 left [3]) and develop new technologies. Fig. 1 shows a demand scenario for nuclear medicine treatments in Europe (2020–2040) measured as number of patient doses ($\times 1000$). The figure contains contribution from a few therapy categories: therapies based on Lutetium-177, other beta-emitting radiopharmaceuticals, targeted α therapy using isotopes such as Actinium-225, Traditional treatments like Iodine-131 and brachytherapy remain relatively constant. The figure highlights a major shift in nuclear medicine toward targeted radiopharmaceutical therapies, which will drive a large increase in therapeutic isotope demand. Most of all it shows a very strong increase in demand for therapies, even almost 3 times during 5 years only (2025-2030).

(left) Demand scenario for various type of therapies [3], (right) the production and the demand of Molybdenum-99 (^{99}Mo) over time (2018-2024) [4].

Fig. 1 (right) shows the production and the demand of Molybdenum-99 (^{99}Mo) over time (2018-2024) [4]. ^{99}Mo is crucial in present medicine because it decays to Technetium-99m, which is used in most nuclear medicine diagnostic scans. In recent years, the production capacity of Molybdenum 99 (Fig. 1 (right, in red) has just been enough to meet the demand (Fig. 1 right, in green) although in some cases (2018) a major crisis took place, when the availability of radioisotopes was much smaller than demand.

This figure shows a clear stagnation in radioisotope production.

Summarizing there is a key trend in nuclear medicine:

- Diagnostic isotope supply (e.g., $^{99}\text{Mo}/^{99\text{m}}\text{Tc}$) is relatively stable and well established, but it barely covers present demand,
- Therapeutic isotope demand is expected to grow rapidly, especially for targeted radionuclide therapies.



Figure 1. Scaffolds fabricated by two-photon polymerization technique for the development of brain models, commercially available from Laser nanoFab GmbH (left) and functional neurons-glia network developed inside these scaffolds (right).

This implies that future production capacity, particularly for therapeutic isotopes, must expand significantly to meet clinical demand in Europe. In this respect laser induced production of short lived isotopes could substantially change the situation. Lasers that could operate near hospitals and provide easy and fast access to short-lived isotopes.

In this context, in recent experiments with the VEGA-3 laser at CLPU (Centro de Láseres Pulsados) in Salamanca, Spain, we demonstrated the feasibility of producing ^{43}Sc , ^{44}Sc , ^{48}Sc , ^7Be , ^{11}C , and ^{18}F using laser-accelerated particles, achieving yields up to $\sim 10^6$ nuclei per shot. With higher repetition rates and optimized targets, such systems could evolve into compact, hospital-adjacent radionuclide sources

In the experiment, we used a pitcher–catcher set-up: a laser-irradiated foil (pitcher) generates protons via Target Normal Sheath Acceleration (TNSA), which then strike a separate target (catcher) of a precursor material to induce nuclear transmutation and the generation of radioisotopes. In this scheme, we also irradiated boron-rich catchers to induce laser-driven hydrogen–boron ($p-^{11}\text{B}$) fusion ($p + ^{11}\text{B} \rightarrow 3\alpha + 8.7 \text{ MeV}$), which produces three energetic α -particles per reaction [5, 6]. This an allow for the generation of intense α -particle sources and then for the generation of different kind of radioisotopes via α -induced nuclear reactions.

Experimental Set-up

The experimental campaigns dedicated to radioisotope production were carried out during two experiments performed at CLPU using the VEGA-3 petawatt laser system. The laser energy before compression was maintained at about 28 J, corresponding to an on-target energy of about 6 J. The pulse duration was tuned between 180 and 280 fs to optimize the proton energy spectrum generated via the TNSA mechanism [7]. For the production of radioisotopes, we used pitcher-catcher configuration (Fig. 2(left)) in accumulation scenario (the pitcher was changed at each laser shot while the catcher was always the same, hence accumulating proton irradiation).

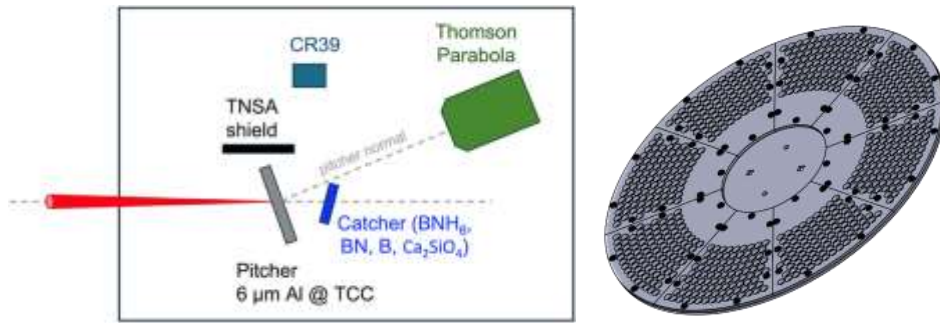


Figure 2. Scaffolds fabricated by two-photon polymerization technique for the development of brain models, commercially available from Laser nanoFab GmbH (left) and functional neurons-glia network developed inside these scaffolds (right).

(left) Experimental setup. (right) Turning wheel that allowed to increase the repetition rate of the operations realized by Instituto Galego de Física de Altas Enerxías, Universidade de Santiago de Compostela, Santiago de Compostela, Spain [8].

A comprehensive set of diagnostics was employed for detection of emitted ions and gamma radiation, including CR-39 nuclear track detectors, a Thomson parabola spectrometer, time-of-flight (ToF) systems and a high-purity germanium (HPGe) detector. Energy-resolved proton spectra were recorded with a Thomson parabola spectrometer coupled to a multi-channel plate or IPs. Proton-induced secondary radiation was analyzed using HPGe γ -ray spectroscopy.

The aim of the first experiment was to prove that laser induced radioisotope production is possible. During the second experiment for the first time, high-repetition-rate operation (0.14 Hz) was implemented, significantly enhancing the overall production yield of the radioisotopes of interest. This mode relied on a rotating wheel [8] containing pitcher targets and enabling rapid change of target between consecutive shots. This allowed us to pass from an accumulation of about 30 shots in the first experiment

to an accumulation of about 300 shots in one series of measurement in following experiment. However, the increased repetition rate led to reduced maximum proton energies, 17.5 MeV measured in the first experiment down to 12.5 MeV.

Results and discussion

In the article showing the results of the first experiment [9, 10], which took place in 2023, we presented a description of the HPGe detector system and described in detail the associated calibration procedure including energy and activity calibration Fig. 3 [9]. The detector sensitivity was calculated on basis of several measurements [9].

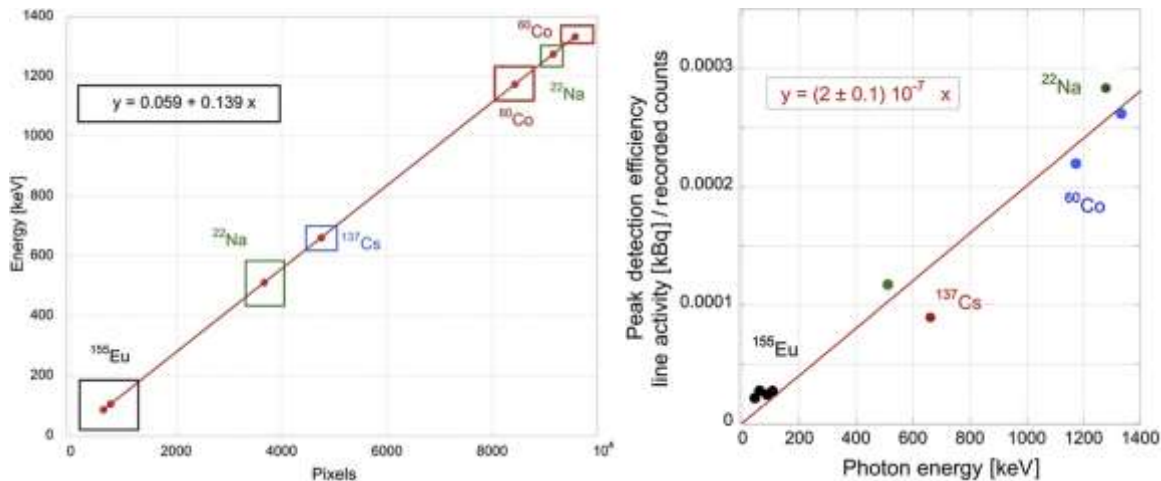


Figure 3. Scaffolds fabricated by two-photon polymerization technique for the development of brain models, commercially available from Laser nanoFab GmbH (left) and functional neurons-glia network developed inside these scaffolds (right).

(left) Energy calibration of the HPGe detector [9] (right) Activity calibration line showing the peak detection efficiency as a function of g-ray photon energy (considering counts recorded during a 5-min acquisition) [9].

We successfully identified γ -ray lines from several radioisotopes produced through irradiation with laser-generated protons. The detected isotopes included ⁴³Sc, ⁴⁴Sc, ⁴⁸Sc emitted using calcium silicate target and ⁷Be, ¹¹C, and ¹⁸F emitted after interaction of proton beam with boron target (Fig. 4, [9]). In addition, we provided an evaluation of how laser-driven particle sources could potentially become competitive with conventional methods for radioisotope production.

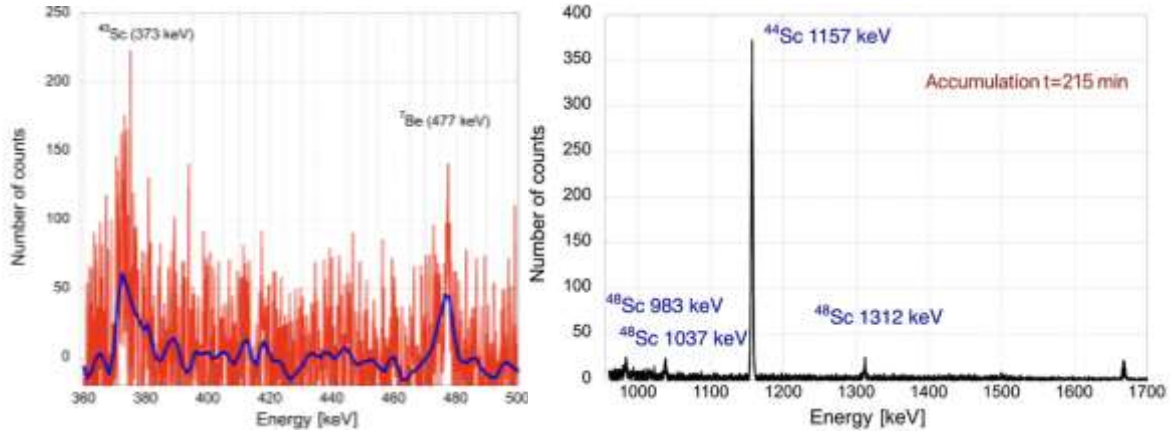


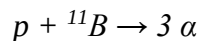
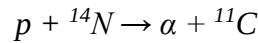
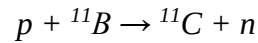
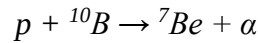
Figure 4. Scaffolds fabricated by two-photon polymerization technique for the development of brain models, commercially available from Laser nanoFab GmbH (left) and functional neurons-glia network developed inside these scaffolds (right).

- Gamma ray spectrum recorded during the first experiment at Vega-3 [9].

Our first measurements demonstrated the production of approximately 6×10^6 of ^{11}C radioisotope and about 5×10^4 of ^{44}Sc radioisotope per laser shot. Furthermore, we demonstrated a good agreement between results obtained from γ -ray spectroscopy and those derived from other diagnostics, such as CR39 detectors. This consistency highlights the potential of γ -ray spectroscopy as a reliable diagnostic tool for quantifying target activation and determining nuclear reaction rates. Such capability is particularly relevant in experiments involving proton–boron fusion, where measuring α -particle yields using CR39 detectors alone has traditionally posed significant challenges [11, 12].

The production yield was substantially enhanced in our second experiment through significant increase of the repetition rate of the measurement. This was achieved by application of a turning wheel [8] which enhanced repetition rate of the measurement to 0.14 Hz. In contrast to the previous experiment where radioisotopes were produced using proton beams in this experiment, we also managed to produce radioisotopes using alpha particle beams.

^{11}C was produced by interaction of the proton beams with a 5 mm thick boron nitride (BN) target and by interaction of alpha particles with a 1 mm thick ammonia borane (BNH_6) target following reactions:



For α -particles, produced by the reaction $p + {}^{11}\text{B} \rightarrow 3\alpha$ as expected, we measured a lower production with the BNH_6 target due to lower boron and nitrogen densities resulting in less nuclear reactions happening. The preliminary results obtained with BN target shows 5.0×10^6 α particles and 1.6×10^7 ${}^{11}\text{C}$ per shot. For BNH_6 target we produced 2.5×10^5 α particles and 1.0×10^6 ${}^{11}\text{C}$ per shot (95 % less than for BN target).

Following interaction of protons with lithium-fluoride (LiF) crystal targets $p + {}^7\text{Li} \rightarrow {}^7\text{Be} + n$, we also measured the production of 1.8×10^7 neutrons per shot.

The main goal of this experiment was to increase amount of detected scandium. Following interaction of proton and α -particle beams with targets containing calcium we detected ${}^{43}\text{Sc}$ and ${}^{44}\text{Sc}$ a few different radioisotopes, increasing the number of generated radioisotopes. Using Calcium silicate target in interaction with proton beams, we produced 10^5 of ${}^{44}\text{Sc}$ atoms per shot.

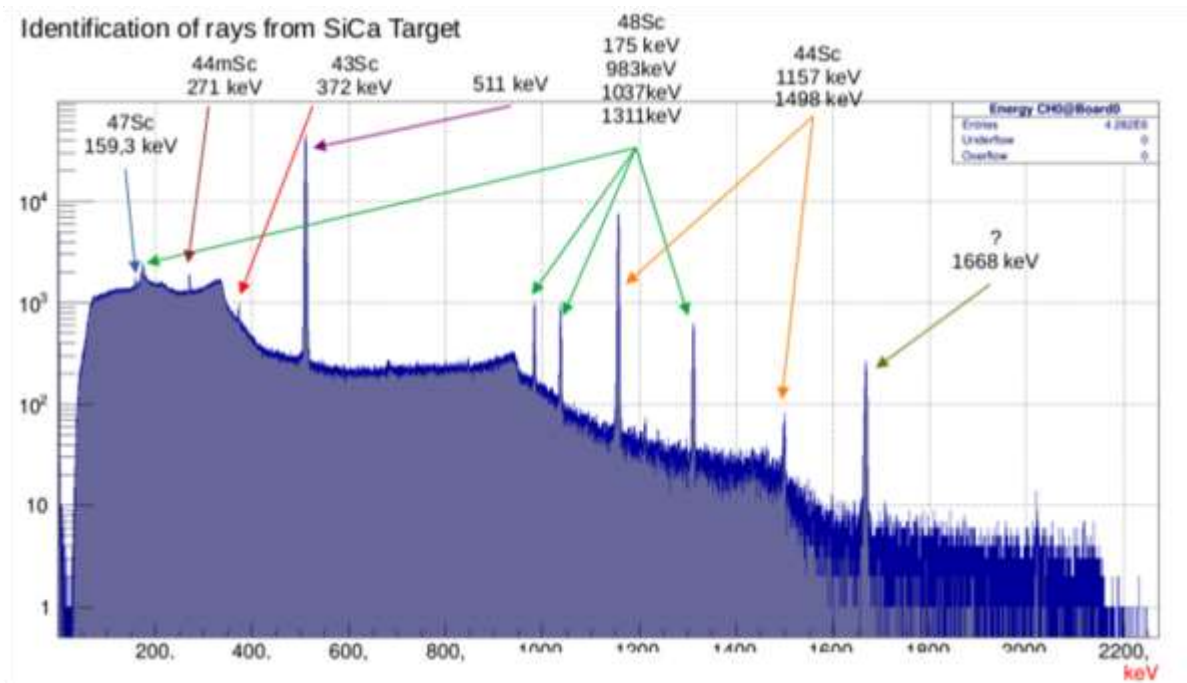


Figure 5. Scaffolds fabricated by two-photon polymerization technique for the development of brain models, commercially available from Laser nanoFab GmbH (left) and functional neurons-glia network developed inside these scaffolds (right).

5. γ -ray lines emitted from the radioisotopes generated using Calcium Silicate (Ca_2SiO_4) target.

Summary

Using the petawatt, high-repetition-rate VEGA-3 laser at CLPU (Salamanca), we demonstrated laser-driven production of radioisotopes via proton- and α -particle-induced nuclear reactions.

In the future, the use of pure ^{11}B targets would improve ^{11}C production, while pure ^{44}Ca targets could significantly increase the yield of ^{44}Sc . These results open promising prospects for the development of laser-driven radiation sources capable of producing medically relevant radioisotopes.

Looking ahead, future work will need to address two key objectives. The first is to perform experiments capable of producing quantities of radioisotopes that can be efficiently separated and collected. The second is to reach activity levels comparable to those required for medical applications, typically in the megabecquerel (MBq) range. Achieving these goals will likely require operating at higher laser repetition rates to accumulate a much larger number of shots, optimizing laser parameters, and developing advanced target designs. In particular, new composite targets could be explored, such as α -particle-producing materials containing boron combined with precursor materials for the desired radioisotopes.

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Toward a Paradigm Shift: Transitioning from Pharmaceutical to Biophysical Approaches in Modern Medicine

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Abstract

For more than a century, the dominance of pharmaceutical-based therapies has shaped the foundations of modern medicine. While drug-based treatments have achieved remarkable success in combating infectious diseases, chronic illnesses, and a wide spectrum of pathological conditions, their limitations—including adverse side effects, systemic toxicity, and the accelerating problem of drug resistance—have become increasingly evident. These challenges highlight the urgent need to explore complementary and alternative therapeutic strategies that can offer higher precision, reduced toxicity, and improved patient outcomes.

This paper aims to develop and apply a comparative analysis framework to evaluate the pharmaceutical and biophysical paradigms across mechanistic, efficacy, safety, and economic dimensions. A structured literature review and conceptual analysis were conducted. Key modalities of biophysical medicine—including nuclear medicine theranostics, magnetic resonance-guided focused ultrasound (MRgFUS), transcranial magnetic stimulation (TMS), and cold atmospheric plasma (CAP)—were systematically compared against standard pharmaceutical interventions. The analysis focused on target specificity, regenerative potential, temporal dynamics, and systemic impact.

The paradigm shift from a predominantly pharmaceutical model toward an integrated biophysical framework underscores a transformative vision for the future of medicine. By combining physics-based methods with clinical expertise, biomedicine may move toward safer, more effective, and personalized therapeutic strategies that reduce dependence on chemical drugs and open new horizons in healthcare.

Keywords: Biophysical Medicine; Pharmaceutical Paradigm; Comparative Analysis; Medical Physics; Precision Medicine; Theranostics; Cold Atmospheric Plasma; Neurostimulation.

1. Introduction

The 20th century was defined by the triumph of pharmaceutical medicine. The discovery of molecules capable of selectively modifying biological pathways—from antibiotics to biologics—revolutionized healthcare. However, this model is increasingly strained by intrinsic limitations: the global crisis of antimicrobial and chemotherapeutic resistance, pervasive systemic toxicity, exorbitant development costs, and a reactive rather than regenerative approach to chronic diseases [1-4]. Recent advances in medical physics have given rise to the field of biophysical medicine, which integrates physical sciences into clinical practice. By leveraging physical principles and advanced technologies, biophysical approaches aim to: (i) minimize chemical side effects, (ii) provide site-specific and personalized interventions, (iii) employ real-time imaging and feedback systems, and (iv) utilize the intrinsic physical properties of cells and tissues for enhanced therapeutic efficacy.

Among the most promising modalities are nuclear medicine, magnetic resonance-based diagnostics and treatments, and neurophysical methods. Particularly noteworthy is laser-plasma medicine, a rapidly emerging field that uses ultra-short laser pulses to generate plasma capable of interacting with biological tissues at the cellular and molecular levels. Applications include targeted cancer cell ablation, sterilization, and wound healing, with minimal damage to surrounding tissues. Cold atmospheric plasma (CAP) therapies, in particular, are demonstrating considerable potential in oncology and dermatology, offering non-invasive and selective treatment pathways.

Concurrently, advances in medical physics have transitioned from providing primarily diagnostic tools to enabling novel therapeutic modalities. Techniques such as targeted radionuclide therapy, MRgFUS, and CAP therapy represent a new frontier—biophysical medicine—that employs controlled physical energy for intervention [5-9]. This paradigm operates on the principle that biological systems are inherently physical, responsive to energy fields, and can be modulated to restore homeostasis without exclusive reliance on molecular agents.

While the promise of biophysical medicine is widely acknowledged, a systematic, head-to-head comparison with the established pharmaceutical paradigm is lacking. Most analyses remain siloed within specific disciplines. This paper seeks to fill this gap by proposing a structured comparative framework and applying it to evaluate the core characteristics, advantages, and limitations of each paradigm. Our central thesis is that biophysical medicine represents a complementary and necessary evolution, shifting the therapeutic logic from chemical inhibition/stimulation to physical modulation and bioenergetic restoration.

2. Methods and Approaches

To conduct a rigorous comparison, we developed a multi-dimensional analytical framework and applied it to a selection of key modalities.

2.1. Analytical Framework:

The paradigms were evaluated across four primary dimensions:

Mechanistic Foundation: The fundamental principle of intervention (molecular binding vs. energy exchange).

Specificity and Systemic Impact: The ability to target diseased tissue while sparing healthy systems.

Temporal Dynamics and Reversibility: The timescale of action and the potential for non-destructive modulation.

Therapeutic Outcome and Regenerative Potential: The capacity to manage symptoms versus promote structural repair.

2.2 Data Collection and Synthesis

A narrative but systematic literature review was performed using major scientific databases (PubMed, Google Scholar, Web of Science) for publications from 2010 to 2024. Search terms included "biophysical medicine," "plasma medicine," "theranostics," "pharmaceutical limitations," "drug resistance," combined with modality-specific terms. Foundational papers and high-impact clinical trials were prioritized. Data on efficacy, side effects, costs, and mechanisms of action were extracted and synthesized for a comparative analysis. Detailed visual representation of our research methodology and its workflow is given by the a blockchain-inspired figure 1; simplified visual representation – figure 2.

Detailed Blockchain Workflow Diagram

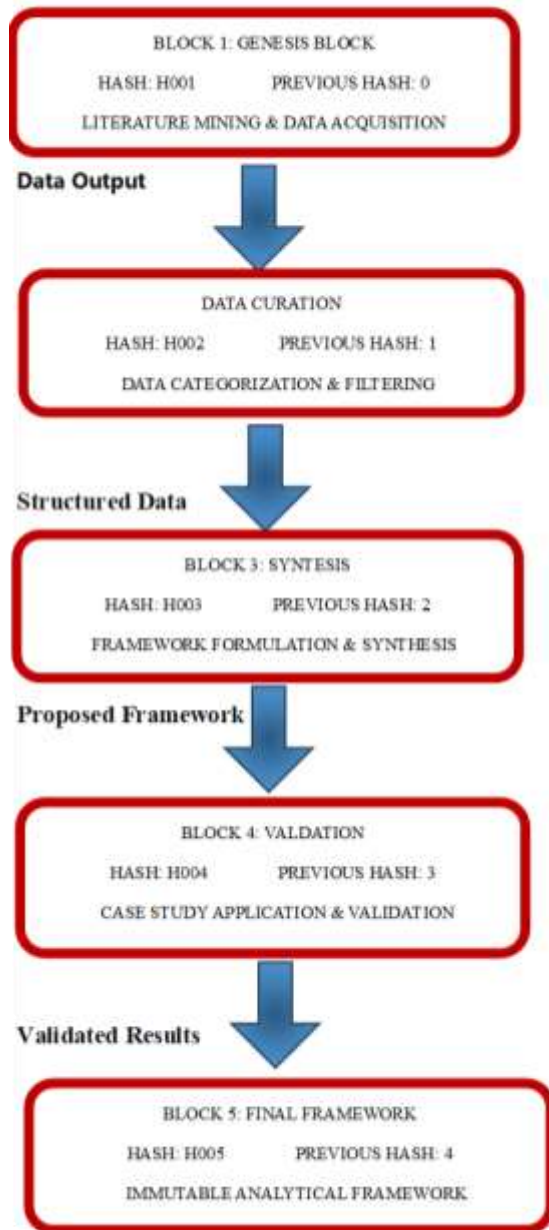


Figure 1: Detailed Blockchain Workflow Diagram. A blockchain-inspired schematic representing the structured, iterative, and verifiable process of the comparative analysis between pharmaceutical and biophysical paradigms. This diagram visualizes our analytical methodology as a chain of interconnected "blocks," where each block represents a phase of data processing, and the "hashes" ensure the integrity and logical connection between stages. The process begins with raw data input and culminates in the final, validated analytical framework.

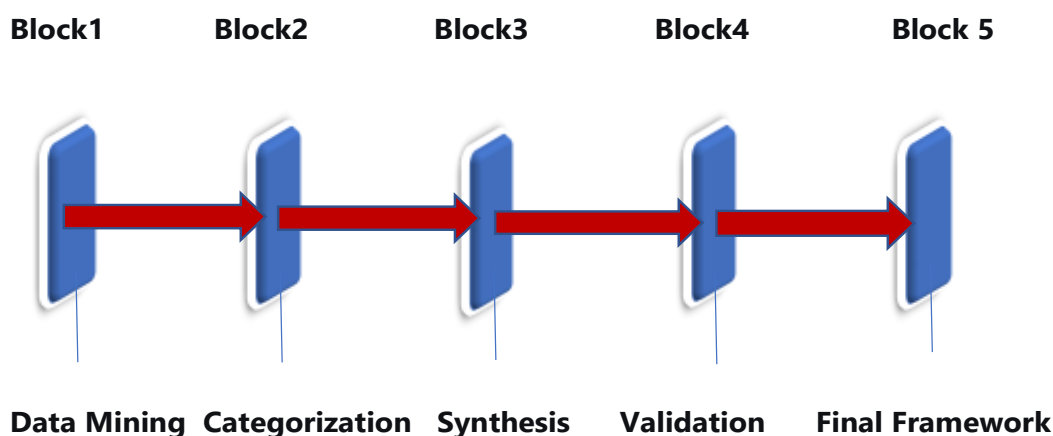


Figure 2: Simplified Visual Representation. A schematic of this iterative and verifiable methodology is presented for illustration of the process using a blockchain-inspired workflow to emphasize data integrity and logical progression.

3. Results: A Comparative Analysis

The application of our framework yielded clear distinctions between the two paradigms, summarized in Table 1.

Table 1. Comparative Analysis of Pharmaceutical vs. Biophysical Paradigms

Dimension	Pharmaceutical Paradigm	Biophysical Paradigm
Mechanistic Foundation	Chemical binding to receptors/enzymes	Energy transfer (EM fields, radiation, plasma)
Target Specificity	Biochemical affinity; often systemic diffusion	Spatial focusing via imaging/field guidance
Systemic Toxicity	High (off-target binding)	Low (localized energy deposition)
Temporal Dynamics	Slow, requires sustained concentration	Instantaneous/short-term; often tunable
Regenerative Potential	Low (primarily symptomatic)	High (stimulates repair mechanisms)
Development Cost	Very High (~\$2B/drug) [2]	High initial R&D, lower marginal cost
Personalization	Limited (weight-/age-based dosing)	High (real-time feedback and dosimetry)

3.1 Illustrative Case Studies:

Oncology: Chemotherapy vs. Cold Atmospheric Plasma (CAP): Chemotherapy acts systemically, damaging rapidly dividing cells indiscriminately, leading to severe side effects. In contrast, CAP generates reactive species that selectively induce apoptosis in cancer cells due to their distinct redox biology, preserving healthy tissue and demonstrating efficacy against multidrug-resistant strains [10].

Neuropsychiatry: SSRIs vs. Transcranial Magnetic Stimulation (TMS): Selective serotonin reuptake inhibitors (SSRIs) modulate neurotransmitter levels throughout the brain over weeks, causing various systemic side effects. TMS uses focused magnetic fields to non-invasively modulate activity in specific cortical circuits (e.g., the dorsolateral prefrontal cortex for depression), achieving comparable efficacy with a markedly different side-effect profile [11].

Tissue Repair: Growth Factors vs. Pulsed Electromagnetic Field (PEMF) Therapy: Topical growth factor applications are costly and can have variable efficacy. PEMF therapy applies specific electromagnetic fields to promote bone and soft-tissue regeneration by enhancing endogenous calcium signaling, nitric oxide production, and angiogenesis, demonstrating a cost-effective, non-invasive regenerative strategy [12].

4. Discussion and results

The pharmaceutical paradigm, while transformative, faces significant limitations including drug resistance, systemic toxicity, and high costs. Biophysical medicine, which utilizes physical energy (e.g., electromagnetic fields, plasma, radiation) for therapeutic purposes, emerges as a complementary and potentially disruptive paradigm. A systematic comparison of these frameworks is needed. The analysis demonstrates that biophysical modalities offer superior spatial specificity and reduced systemic toxicity through localized energy delivery. They exhibit unique capacities for stimulating endogenous regenerative processes, a feature largely absent in pharmacology. Furthermore, biophysical interventions often allow for real-time feedback and adaptive control, enabling a higher degree of personalization. However, they face challenges in dosimetry standardization and require significant upfront technological investment.

The biophysical paradigm does not merely replace but fundamentally complements the pharmaceutical model. It represents a shift from chemical correction to physical modulation and bioenergetic restoration. A hybrid, synergistic approach, leveraging the strengths of both paradigms, is

identified as the most promising trajectory for future medicine. This transition necessitates concurrent evolution in regulatory frameworks and medical education.

Our analysis confirms that the biophysical paradigm offers distinct advantages in specificity, personalization, and regenerative capacity. Its foundational principle—**control through energy**—allows for interventions that are spatially confined and adaptable in real-time, aligning perfectly with the goals of precision medicine.

However, this shift is not without challenges. The "dose" in biophysical medicine is a complex function of energy, time, and tissue properties, requiring sophisticated modeling and monitoring—a stark contrast to the mg/mL standardization of drugs. This necessitates the development of new regulatory science focused on energy dosimetry and device-biocompatibility. Furthermore, the high initial cost of biophysical technologies and the need for specialized training risk creating a new form of healthcare inequity.

The most promising path forward is not a replacement but a **synergistic integration**. The emerging field of hybrid theranostics exemplifies this: a radiopharmaceutical is used both to image (diagnose) and to deliver targeted radiation (therapy). Similarly, plasma-activated liquids can sensitize tumors to conventional chemotherapy, and ultrasound can transiently open the blood-brain barrier for targeted drug delivery. These approaches leverage the molecular specificity of pharmacology and the spatial precision of physics.

5. Conclusion

This comparative analysis demonstrates that biophysical medicine represents a profound and necessary evolution in therapeutic strategy. It addresses critical limitations of the pharmaceutical model, particularly concerning toxicity, resistance, and the lack of regenerative impetus. The paradigm shift is from seeing the body as a set of molecular locks requiring chemical keys, to viewing it as a dynamic, energy-information system that can be tuned and reset.

The future of medicine lies in a unified framework that intelligently combines the best of both worlds: the systemic reach and molecular precision of drugs with the localized, regenerative, and personalized potential of biophysical modalities. Realizing this future will require concerted efforts in interdisciplinary education, the development of new regulatory pathways, and a commitment to ensuring equitable global access to these transformative technologies.

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Study of Pathogenic Microorganisms by Optical Spectrometry Methods

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Keywords: Spectra, Spectrometry, Scattering, Simulation, Virus-like particles.

Abstract

Modern detection and identification systems of pathogenic microorganisms are based on biochemical and biophysical methods, immune-enzymatic and serological analysis, PCR testing and others. Currently, ultraviolet (UV), visible-infrared (Vis-IR), and Raman spectroscopy are widely employed for spectral analysis of bio-materials. Challenges encountered during experimental studies include issues with sample preparation, low signal intensity, the accuracy of measuring instruments, and the processing of spectroscopy data. Infected biological samples, particularly bio-fluids like blood, saliva, tears, urine, and sweat contain recognized biological markers such as lipids, peptides, tryptophan, tyrosine, and cortisol, among others. Spectrometers determine the spectra associated with specific bonds, molecules or functional groups within various substances. Optical spectrometry methods enable the determination of the scattering or absorption spectra of pathogenic microorganisms. Our research focused on the scattering properties of bio-particles and the relation of scattering intensity with the wavelength of the excitation source. The resonance wavelength ranges are determined using both empirical formulas and theoretical models. Our approach views the bio-sample as a micro/nano system comprised of bio-particles that contain pathogenic microorganisms and exist in different phases - solid, liquid, or gaseous. The results obtained are based on a simulation method and classical electrodynamics boundary problem solutions. Spectra of viral bio-particles are proposed for consideration. Our findings indicate that the resonance scattering wavelengths for viral particles are predominantly observed within the UV range.

Introduction

Pathogenic microorganisms are fascinating and multifaceted objects of study of microbiology, molecular biology, bioscience, and biotechnology. The world of these organisms is incredibly diverse, encompassing bacteria, viruses, chlamydia, rickettsia, and fungi, referred to as bioagents that cause diseases. Comprehensive study of these micro/nano organisms, particularly in terms of their identification and detection, is crucial for disease prevention and healthcare. Those research is essential for the development and enhancement of modern detection systems and technologies as well.

Microorganisms consist of a variety of bioforms, distinguished from other biological entities by their diverse cellular, molecular, structural, and physicochemical characteristics. This diversity presents challenges for various scientific disciplines, necessitating multidisciplinary research and innovative approaches. Combining biochemical and biophysical research methods with modern tools, computers, and AI technologies is essential for advancing our understanding in this field.

Contemporary detection and identification systems for pathogenic microorganisms utilize biochemical and biophysical methods, including immune-enzymatic assays, serological analysis, PCR testing, and others [1-3]. Direct and indirect detection methods are commonly used in pathogen identification systems. Indirect detection methods, such as virus isolation, provide opportunities for further analysis and characterisation of viruses, thereby improving existing analytical techniques. On the other hand, direct detection methods utilise modern technologies, including nucleic acid and immunological detection [3]. While some of these methods offer high sensitivity, they can also be time-consuming, costly, and may require amplification systems, specialised equipment, trained personnel, and specific point-of-use applications.

For the rapid and effective detection and identification of pathogens, in the current decade, especially following the COVID pandemic, the development of various approaches and technologies, along with the improvement of existing methods, has become increasingly relevant. Among these, spectroscopic methods and modern spectroscopic equipment, including portable spectrometers, are noteworthy [4-14]. Spectroscopy of pathogens and bio-materials enables the determination of spectral signatures, which are the most relevant identification features of materials, compositions, molecules, and atoms. Currently, ultraviolet (UV), visible-infrared (Vis-IR), and Raman spectroscopy, along with their modifications and enhanced methods, are extensively utilized for the spectral analysis of biological materials, including bio-molecules, cells, tissues, bacteria, and viruses [4-16]. Spectrometers determine the spectra associated with specific bonds, molecules or functional groups within various substances.

Analyzing and comparing spectra is an effective method for identifying molecules and composites, and it should also be used for identifying unknown pathogenic materials. To facilitate this process, it is essential to have databases that contain spectral signatures of various biomolecules and biospecies. Another approach for detecting pathogens and viruses in experimental samples involves comparing the spectra of healthy materials with those of virulent ones. Infected biological samples, particularly bio-fluids like blood, urine, tears, saliva, and sweat contain recognized biological markers such as peptides, tyrosine, tryptophan, lipids, and cortisol, among others.

Challenges encountered during experimental studies include issues with sample preparation, low signal intensity, the accuracy of measuring instruments, and the processing of spectroscopy data. When conducting spectroscopic experiments, in addition to selecting the components of the experimental device (setup), the expected range of absorption or scattering spectra of the test samples, sample concentration, physical and chemical properties of the environment, solution, or target glass/cuvette material, their transparency, etc., should be taken into account.

In contemporary research, the processing of spectroscopy data involves a variety of advanced analytical methods. It includes the meticulous analysis of raw spectral data through techniques such as baseline correction, noise reduction, and signal enhancement. Additionally, the integration of sophisticated software tools facilitates the interpretation of complex datasets, allowing for more accurate identification of chemical compounds and their concentrations. Furthermore, the application of artificial intelligence technologies, such as machine learning algorithms, enables automated pattern recognition and predictive modelling, significantly improving the efficiency and accuracy of data analysis.

Optical spectrometry methods enable the determination of the scattering or absorption spectra of pathogenic biomaterials, including viruses. It is known that Raman spectroscopy originates from electromagnetic (EM) waves/light and particle scattering, namely, the inelastic scattering. It can directly probe vibration or rotational states in molecules [11]. Infrared (IR) spectroscopy provides information about molecular vibrations and corresponding absorption and IR-active spectra [17, 18]. Both scattering and absorption result from the interaction between an electromagnetic (EM) wave and a substance, material, or particles. Scattering and absorption leads to the redistribution of energy of EM wave. Scattering involves the deflection of the EM wave in various directions due to irregularities or small particles in the medium, while absorption refers to the process where the wave's energy is taken up by the material, often resulting in the conversion of that energy into heat.

Characterising and analysing resonant scattering and absorption of EM waves is essential for studying the optical and spectroscopic properties of materials and particles of biological or non-biological origin. Our research focused on the resonant scattering properties of pathogenic microorganisms, especially viruses using spectrometry and mathematical modelling methods for estimation the resonant ranges and scattering intensity of bio-particles, and the relation of characteristics versus wavelength of the excitation source.

Method of decision

It is well known that a material and a particle absorb and reflect the energy of the incident field, and it is the result of the interaction of electromagnetic (EM) field and the material/particle. Estimation of absorption, reflection or scattering capabilities is possible using physical, theoretical or numerical methods [19-22]. Measuring or computing techniques are applied to determine the specific physical characteristics. Modern optical setups are well-adapted to measuring and amplifying scattering signals. As noted by Bohren and Huffman, the detector "sees" only the scattered light [19]. Therefore, detection and estimation of scattering signals for studying optical (scattering) properties of materials/particles is essential for the characterisation of particles, especially particles of biological origin.

One of the measurable quantities that characterises the response to EM waves (signal) & particle interaction is the physical quantity called Scattering Cross Section (σ). It emphasises the conservation of energy aspect of extinction and is associated with the Poynting vector ($\vec{P}$), representing the power flow of an EM field. Based on relation $w_s = \int_s P_r ds$, we able to estimate energy flux per area s (per unit time) and accordingly, the Total (Extinction) Cross Section $\sigma = \sigma_{scatt} + \sigma_{abs}$, where σ_{scatt} and σ_{abs} denote the cross sections corresponding scattering and absorption ability, P_r is Poynting vector component normal to surface. In a non-absorbing medium, the total scattering cross section can be expressed as the ratio of the energy flux of the scattered (in all directions) waves (w_{scatt}) to the energy flux of the incident waves (w_{in})

$$\sigma_T = \sigma_{scatt} = \frac{w_{scatt}}{w_{in}} . \quad (1)$$

Another characteristics of a scattering wave are the Differential Scattering Cross Sections (Forward and Backward), which specify the angular distribution of the scattered energy into a unit solid angle about a given direction [22]

$$\sigma_{diff} = \lim_{r \rightarrow \infty} [r^2 P_{scatt} / P_{in}]. \quad (2)$$

Usually, we consider the monochromatic sinusoidally ($\exp(-i\omega t)$) varying plane wave and the corresponding time-averaged Poynting vector ($\vec{P}$) at any point outside the particle. The analytical expression of the Poynting vector also allows for estimating the intensity (I): $I = \left| \vec{P} \right| = \frac{1}{T} \int_0^T \vec{P} dt$,

where T is the time-period.

In the far EM field zone of a particle ($kr \gg 1$), EM field energy propagation is preferable in the radial direction, and to describe the energy distribution, we should estimate the radial (r) component of the Poynting vector

$$\vec{P}_r = \left[\vec{E} \vec{H}^* \right]_r, \quad (3)$$

where $\vec{E}$ and $\vec{H}$ are electric and magnetic field vectors, correspondingly, k is the wave number in vacuum, * - denotes the complex conjugate. The time-averaged Poynting vector can be expressed through the formula

$$\vec{P}^t = \frac{1}{2} \text{Re} \left[\vec{E} \vec{H}^* \right]. \quad (4)$$

Studying optical properties and estimating the scattering characteristics of materials/particles is linked to the development of theoretical or numerical methods capable of defining the electric and magnetic field components. An elaborated concept and methodology applicable for studying pathogenic microorganisms, namely viruses, is proposed for consideration. Our approach considers the bio-sample as a micro/nano system composed of pathogenic particles that exist in solid, liquid, or gaseous phases. These types of bio-systems, as well as the interaction of EM field & bio-system in different surrounding media, we consider from a physical point of view. It means that bio-systems or bio-particles are characterised by the set of geometric (sizes, shape) and physical (electric and magnetic) parameters.

Based on the concept, classical EM wave theory and modelling methods applied to bio-systems allow us to estimate the scattering characteristics of nano/micro system, identify the ranges of resonance wavelengths, and determine the scattering resonance spectral signature of bio-particles system [23-25].

Let's examine a bio-system consisting of a single viral particle to illustrate the potential of the proposed approach for determining the scattering spectra of a viral particle. In this context, we should consider the physical problem of the interaction of a single viral particle & EM field.

The structure of a large number of virions, the extracellular infective form of a virus, is icosahedral or near-spherical with icosahedral symmetry. Two media of different structures and properties constitute the virion: core containing the nucleic acids (DNA or RNA) and the shell of protein capsomeres, called the capsid. Therefore, we could model the virion as a core-shell structured spherical particle, characterised by outer (d_2) and inner (d_1) diameters of the capsid. Optical properties of the particle are defined by the electric (ϵ_1 and ϵ_2) and magnetic (μ_1 and μ_2) parameters of the core and shell of the virion, correspondingly (Figure 1).

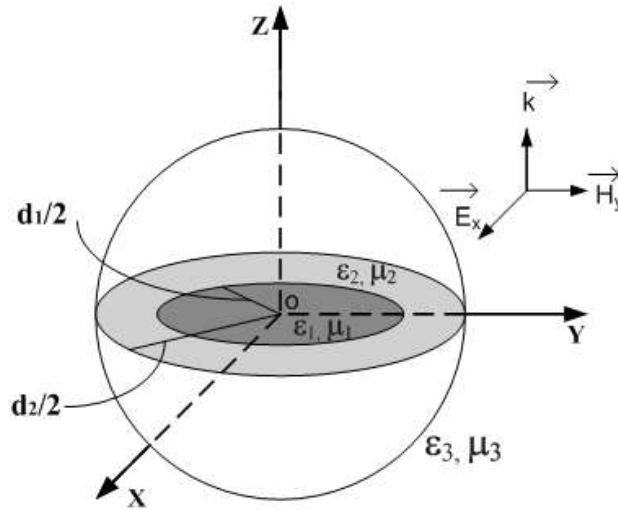


Figure 1. Model of virus-like particle of spherical shape.

Radial component of the Poynting vector (Eq. 3) in spherical coordinate system (r, θ, φ) may be written as

$$\vec{P}_r = \left[\vec{E} \vec{H}^* \right]_r = (E_\theta H_\varphi^* - E_\varphi H_\theta^*) . \quad (5)$$

Accordingly, we can obtain the formula for defining

$$w_s = \int_s P_r ds = \int_s P_r r^2 \sin \vartheta d\vartheta d\varphi = \int_0^{2\pi} d\varphi \int_0^\pi P_r r^2 \sin \vartheta d\vartheta \quad (6)$$

Based on definitions (Eq. 1-Eq. 3), we get analytical expressions of Total Scattering Cross Section (σ_T) and Differential Scattering Cross Sections (Backward - σ_B , Forward - σ_F), which estimate the scattering ability of particles in far-field ($r \gg 2d_2^2 / \lambda$):

$$\sigma_T = 2\pi \frac{1}{k_3^2} \sum_{s=1}^{\infty} (|A_s^e|^2 + |A_s^m|^2) \frac{s^2(s+1)^2}{(2s+1)}, \quad (7)$$

$$\theta = \pi, \quad \sigma_B = \frac{1}{k_3^2} \left| \sum_{s=1}^{\infty} i^s \frac{1}{2} s(s+1) (A_s^e - A_s^m) \right|^2, \quad (8)$$

$$\theta = 0, \quad \sigma_F = \frac{1}{k_3^2} \left| \sum_{s=1}^{\infty} i^{-s} \frac{1}{2} s(s+1) (A_s^e + A_s^m) \right|^2, \quad (9)$$

where, k_3 is the wave number of environment outside the particle. We use notions: $k_q = k\sqrt{\varepsilon_q \mu_q}$ in the (q) medium, (ε_q) is the electric permittivity, (μ_q) is the magnetic permeability. Coefficients - A_s^e, A_s^m corresponding electric and magnetic modes of EM field are defined by solving the problem using physical and mathematical approaches.

The theoretical solution of the physical problem related to the mentioned scenario is based on classical Maxwell's electromagnetic theory. The separation of variables method [26] and Debye Potentials used for solving Helmholtz's wave equation, lead to the solutions of Bessel's and Legendre's equations in a spherical coordinate system [27]. We represent the electromagnetic field vector components of $\vec{E}$ and $\vec{H}$, in the areas of the shell, core, and surrounding media as sums of multipole waves [20, 28]. The coefficients A_s^e, A_s^m of multipole waves are determined by applying the electrodynamics boundary conditions. As a result of complex mathematical transformations, we obtain a rigorous deterministic solution to the physical problem. Multipole wave coefficients are defined in a precise mathematical form, with combinations of Riccati-Bessel Spherical and Associated Legendre functions, as well as their derivatives [28]:

$$A_s^e = \frac{i^{s-1}(2s+1)}{s(s+1)} \frac{[G_s^e(k_3 b, k_2 b) L_s^e(k_1 a, k_2 a) - L_s^e(k_3 b, k_2 b) G_s^e(k_1 a, k_2 a)]}{\Lambda_s^e(k_3 b, k_2 b) G_s^e(k_1 a, k_2 a) - \Gamma_s^e(k_3 b, k_2 b) L_s^e(k_1 a, k_2 a)} \quad (10)$$

$$A_s^m = \frac{i^{s-1} \frac{2s+1}{s(s+1)} [G_s^m(k_3 b, k_2 b) L_s^m(k_1 a, k_2 a) - L_s^m(k_3 b, k_2 b) G_s^m(k_1 a, k_2 a)]}{\Lambda_s^m(k_3 b, k_2 b) G_s^m(k_1 a, k_2 a) - \Gamma_s^m(k_3 b, k_2 b) L_s^m(k_1 a, k_2 a)} \quad (11)$$

Eqs. 10 and 11 enable us to express the EM field components in terms of analytical functions. Analysis shows that arguments of those functions and scattered field characteristics may be defined in terms of dimensionless size parameters, namely the ratio of particle diameter to wavelength. It makes it possible to consider the solutions for specific cases: Rayleigh Scattering ($\pi d / \lambda \ll 1$), Mie scattering ($\pi d / \lambda \approx 1$), dipole ($d / \lambda \approx 10^{-3}$) and geometric optics approximations ($\pi d / \lambda \gg 1$).

Our research focused on studying the scattering properties of viral particles within wavelength range ($\pi d / \lambda < 1$), which is more specific and prominent for particle characterization. The resonance wavelength range is determined using both the theoretical model and the empirical (computing-based) formula. The upper limit of the resonance range depends on the electric, magnetic, and size parameters of the particle, defined by the formula $\lambda_{\max} < \pi \bar{d} \sqrt{|\epsilon_q \mu_q|}$, and is specific to each one.

Results

Computer simulation and mathematical modelling methods are based on theoretical findings and analytical solutions [28], by applying Eqs. 7-11. We studied the relation of the scattering characteristics of viral particles versus the wavelength of the incident (excitation) wave ($E_x^{in} = E_0 e^{-i\omega t + ik_3 z}$). The simulation “spectra” of the viral particle modeled the virion of bacteriophage T7 is obtained in the MATLAB environment. The number of terms of the sums (Eqs. 7-9) is estimated within a given accuracy (10^{-11}). Size and shape parameters of the T7 icosahedral virion are gained from the databases [29]. Dielectric parameters of DNA and the T7 virion capsid have been experimentally measured using ultra weak polarization forces [30, 31]. “Spectra” in Figure 2 represents the scattering properties in the far-field of the target viral particle (T7) within the resonance scattering range $25 \div 80$ nm. Comparison within equal λ intervals, the number of maxima decreases as λ increases. We can observe that the maximums of scattering cross sections -Total, Forward and Backward almost coincide. Scattering in far zone is mostly more intense in the forward direction than in the backwards direction. Analysis of simulation results indicates that the response of particle & wave interaction, expressed in scattering spectra as a scattering cross-section, strongly depends on the geometric and electromagnetic parameters of the virion [23, 28].

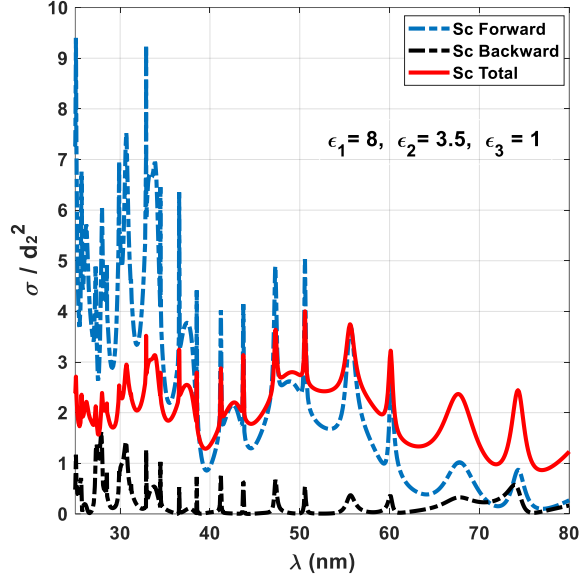


Figure 2. Scattering Cross Sections: Scattering Forward (blue), Scattering Total (red), Scattering Backward (black), diameters of particle: inner $d_1=42.6$ nm, outer $d_2=56.6$ nm, dielectric permittivities: of core $\epsilon_1=8$, shell $\epsilon_2=3.5$, surrounding medium $\epsilon_3=1$; magnetic permeabilities: of core $\mu_1=1$, shell $\mu_2=1$, surrounding medium $\mu_3=1$; Range of wavelength 25÷80 nm.

In this paper, we emphasize the dependence of scattering spectra on the parameters of the environment surrounding the viral particle. Commonly, viral particles are observed in biological fluids produced by the human body, such as sweat. For simulation purpose we use the real part ($\epsilon_{\text{Real}} > \epsilon_{\text{Im}}$) of dielectric permittivity of sweat, which is about to 3,8 - 4,0 at 2.5 THz, measured by terahertz time-domain spectroscopy system [32]. As noted, both the real and imaginary parts of the dielectric permittivity of sweat samples obtained from different body regions decrease with increasing frequency [32]. The dielectric permittivities of vacuum ($\epsilon = 1$) and water ($\epsilon = 1,77$) in the visible light range (600 THz, 500 nm) are use in our simulations. In Figure 3, we present the scattering cross sections -Total (Fig. 3A) and Forward (Fig. 3B) - of the T7 virion for vacuum, water, and human sweat samples. The intensity of forward scattering in a given wavelength range is higher even in different environments. An analysis of the scattering abilities of the T7 virion reveals a clear dependence on both the wavelength and the surrounding environmental conditions. This variation highlights how these factors influence the characteristics of the scattering phenomenon observed.

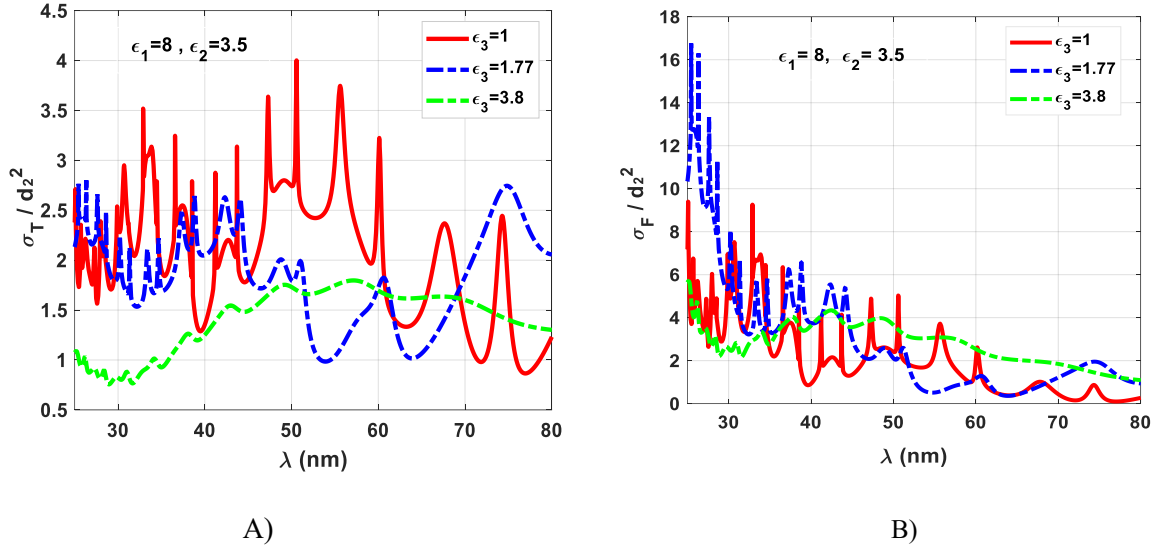


Figure 3. Scattering Cross sections: Total (σ_T/d_2^2) (left, A) and Forward (σ_F/d_2^2) (right, B). Diameters of particle: inner $d_1=42.6$ nm, outer $d_2=56.6$ nm, dielectric permittivities: of core $\epsilon_1=8$, shell $\epsilon_2=3.5$, surrounding mediums $\epsilon_3=1$ (red), $\epsilon_3=1.77$ (blue), $\epsilon_3=3.8$ (green); magnetic permeabilities: of core $\mu_1=1$, shell $\mu_2=1$, surrounding medium $\mu_3=1$; Range of wavelength 25 ÷ 80 nm.

Conclusion

Optical spectrometry methods, based on classical electromagnetic wave theory, are employed, along with modelling and computer simulation techniques, to investigate the scattering or absorption properties of pathogenic microorganisms, specifically viruses. Proposed approach views the bio-sample as a micro/nano physical system comprised of viral particles, characterised by geometric and electromagnetic parameters. A simulation study was conducted for a virus-like particle of specific size and electromagnetic parameters, corresponding to the bacteriophage (T7) virion. The expected spectral response on particle & EM field interaction is clearly observed, in the resonance range, through far-field characteristics such as scattering cross sections. Analysis of results indicates that scattering properties of the particle, in the resonance wavelength range, strongly depend on electromagnetic properties of virus structural parts, such as core (DNA) and shell (proteins), as well as on dielectric permittivities of the surrounding particle medium. The resonance scattering spectra of viral particles are observed within the Ultraviolet range. Scattering “spectra” may be associated with spectral “signatures” of viral particles. Our findings makes it possible to expand the research methods for studying spectral properties of nano- and micro-sized particles (or samples) of organic, inorganic or hybrid origin, structured in spherical or cylindrical shapes. The outcomes derived from theoretical research and simulation studies, in conjunction

with experimental spectroscopy investigations, can be effectively utilised in the fields of disease diagnostics, microbiology, and biotechnology.

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Boron Isotopes Based Neutron Detectors – A Review

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Abstract. The two stable isotopes of boron, ^{10}B and ^{11}B , differ significantly in their neutron capture cross sections: for thermal neutrons, they are 3837 and 5 b, respectively. The high neutron capture cross section of ^{10}B nuclei, combined with its monotonic dependence on neutron energy, makes structural modifications of boron, as well as compounds and composites with high boron content, very attractive not only as materials for nuclear reactors but also for the development of efficient neutron detectors. The concept of neutron detectors and sensors based on boron isotopes is presented based on a literature review of their operating principles, designs, and characteristics.

1. Introduction

The principles of radiation interactions with matter can be utilized to measure ionizing as well as neutron radiation characteristics with detectors or accurately predict radiation fields via Monte Carlo type simulations. The book chapters [1, 2] and presentation [3] are examples of overviews of such kind methods and techniques applied in radiation dosimetry.

1.1. Types of radiation detectors

The main types of radiation detectors are:

- *Gas-filled detectors* (the most commonly used for counting) operating principle is that radiation causes ionization of the gas between two electrodes in the chamber, and the resulting electrical charge is collected as a current pulse.

- *Scintillation detectors* operate on the principle that in response to excitation caused by radiation, certain inorganic or organic materials emit light, i.e., scintillate, due to de-excitation of the crystal lattice or molecules.
- *Semiconductor detectors* consist of semiconducting crystals that absorb radiation energy, transferring electrons from the valence band to the conduction band, which in turn leads to the formation of holes. These electrons and holes are collected by applying an electric field to the detector crystal, causing them to be attracted to the positive and negative electrodes, respectively.
- *Thermoluminescent dosimeters* utilize electron traps in semiconducting crystals to store the radiant energy absorbed by the crystal and detect radiation.
- *Film dosimeters* contain a photographic emulsion, typically composed of silver halide crystals and gelatin, deposited on a transparent polyester base. Incident radiation elevates electrons in the crystals from the valence band to the conduction band. Some of these electrons are captured by electron traps and a weakly negative electric field is generated around their region, attracting a small number of positively charged, mobile interstitial silver ions. They combine with the captured electrons and reduce to metallic silver. The combination of all these metallic silver atoms throughout the film forms a latent image. The film can be developed by chemically removing unexposed grains portion. Consequently, the optical density of the film relates to the received radiation dose.
- *Chemical and gel dosimeters* are based on chemical changes in substances resulting from ionization. For example, Fricke dosimeters are aqueous solutions of ferrous ions Fe^{2+} . Ionizing radiation causes reactions, resulting in their conversion to ferric ions Fe^{3+} . Since the number of converted ions is related to the radiation dose absorbed by the solution, the received radiation can be determined. Other chemical dosimeters are based on polymerization or coloration reactions.
- *Particle track detectors* register particles by etching their tracks, which is possible in some polymers and glasses: during (electro) chemical processing, atomic sites damaged by irradiation with high linear energy transfer particles become visible.

Dosimeters based on optically stimulated luminescence, direct ion storage, calorimetry, radiophotoluminescence, Cherenkov radiation, etc. are also used.

1.2. Detection of neutrons

Most radiation sources that emit X- and/or γ -rays also emit neutrons. Neutron radiation is particularly dangerous to the human body, as the energy loss in tissues creates an intense ion-path. Other

types of radiation, such as β -rays, protons, α -particles, etc., can be generated as a result of its interaction with biological matter. This is why nuclear power plant workers are vulnerable to occupational exposure to neutrons.

It should be noted that since neutrons have no electrical charge and are not ionizing particles, the radiation detectors listed above are not directly suitable for their detection. For example, in the photographic film method standard version, the latent images converted into metallic silver appears as darkening, the degree of which, called the optical density, is too weak to be used for neutron irradiation monitoring. Neutron dosimetry with the film badge utilizes the special neutron-sensitive emulsions, in which the tracks of recoil protons from the scattering of fast neutrons could be analyzed. Similarly, the track technique is widely used in neutron dosimetry: the tracks of the charged recoil particles produced by neutrons can be registered.

In general, neutron detection is accomplished by measuring the charged particles released in nuclear reactions as a result of neutron inelastic or elastic interactions with certain elements. According to the neutrons kinetic energy K , there are slow or thermal ($K < 0.5$ eV) and intermediate speed (0.5 eV $< K < 0.1$ MeV) and fast ($K > 0.1$ MeV) neutrons detection methods.

For slow neutrons, detection is usually the only requirement. Thermal neutron detection is the measurement of their reaction products with ^3He , ^6Li , or ^{10}B nuclei. In particular, the capture of thermal neutrons by the boron ^{10}B nucleus has a high cross section for the reaction $^{10}\text{B}(n, \alpha)^7\text{Li}$, which produces lithium ^7Li , α -particle, and either 2.31 (96%) or 2.79 MeV (4%) of energy E . List these most important nuclear reactions for slow-neutron detection – see the Table 1.

Table 1. Important nuclear reactions for slow-neutron detection.

Reaction	Energy E , MeV	Cross section, b
$^2_3\text{He} + ^1_0\text{n} \rightarrow ^1_1\text{H} + ^1_1\text{H}$	0.765	5330
$^3_6\text{Li} + ^1_0\text{n} \rightarrow ^1_3\text{H} + ^2_4\text{He}$	4.78	940
$^{10}_{10}\text{B} + ^1_0\text{n} \rightarrow ^3_7\text{Li}^* + ^2_4\text{He}$ (96%)	2.31	3840
$^{10}_{10}\text{B} + ^1_0\text{n} \rightarrow ^3_7\text{Li} + ^2_4\text{He}$ (4%)	2.79	3840

Here the cross sections are given for capture of thermal (0.025 eV) neutrons and to distinguish it from the ground state ^3_7Li , the excited state is marked with an asterisk: $^3_7\text{Li}^*$. Since the incident kinetic energy K of a thermal neutron is negligible, the sum of the reaction-products kinetic energies is almost equal to the reaction energy E itself.

Slow-neutron-induced fission (n, f) of ^{233}U , ^{235}U , or ^{239}Pu nuclei is utilized in so-called fission counters. The E value of ~ 200 MeV for each of them is large. About 165 MeV of this energy is converted directly into the heavy fission fragments kinetic energy. Consequently, fission pulses are extremely large, enabling slow-neutron counting to be done at low levels, even in a high background. Commonly, the fissile material is coated on the ionization chamber inner surface. Main disadvantage of using these fissionable materials in neutron detectors is that they are α -emitters, and one must contend with the pileup of α -particle pulses.

Alternatively, the activation foils can be used. Slow neutrons captured by nuclei induce radioactivity in a number of metals (including Mn, Co, Cu, Ag, In, Dy, and Au), which can be made into foils for neutron detection. The amount of induced radiation depends on a number of factors: element chosen, foil mass, the neutron energy spectrum and capture cross section, and the time of irradiation.

The interaction cross sections of ^3He , ^6Li , and ^{10}B isotopes are generally too low for intermediate speed and fast neutrons to allow efficient counting. Besides, for them the energy spectral measurements are frequently needed. Corresponding detectors operate either by slowing the neutrons down to thermal energies prior to detection by use of a moderator or through detection based on other nuclear reactions or elastic scattering alone. The point is that the elastic recoil energies for slow neutrons are negligible, while at higher speeds neutrons can transfer detectable kinetic energies to nuclei (especially hydrogen) through elastic scattering.

In the first method, the detectors again are based on one of the designs used to measure slow neutrons. However, detector is surrounded by a layer of hydrogen-rich moderator material (such as paraffin). Two principal systems in this category have been developed: cylindrical long counter and moderating spheres enclosing a small thermal-neutron detector. Increasing the moderator thickness, on the one hand, improves efficiency by further slowing the neutrons due to the longer path length, but, on the other hand, reduces efficiency, as some neutrons are absorbed by the moderator or deflected before reaching it. Therefore, both the optimal moderator thickness and the detector efficiency (at a fixed moderator thickness) depend on the neutron energy.

In the second method, neutron detectors do not rely on moderation, but on reactions directly caused by the interaction of intermediate speed and fast neutrons, allowing the energy of the interaction products to be measured and used for spectroscopy.

An alternative commercially available method for neutron detection is the superheated droplet dosimetry, which utilizes the bubble chamber concept to detect particles with microscopic (~ 100 μm)

droplets of superheated liquid in a polymer gel matrix. Neutrons passing through the microbubbles impart sufficient energy to vaporize them, forming visible bubbles, the number of which is related to the neutron dose. The advantages of bubble dosimeters include high specificity for neutrons in mixed gamma–neutron radiation field and the ability to be reused by creating excess pressure in the gel. By varying the number of microbubbles in the gel, sensitivity can be varied. Bubble dosimeters are used for neutron dosimetry in medicine, particularly in LINAC (LINear ACcelerator) bunkers, and also as personal dosimeters due to their relatively small size.

Today, a number of companies produce various types of radiation detection systems. One example is Baltic Scientific Instruments (BSI) [4], headquartered in Riga, Latvia, which specializes in the development and manufacture of spectrometric analysis devices based on semiconductor and scintillation radiation detectors. Its radiation sensors and detectors are used in nuclear energy industry, environmental monitoring, geophysics and mining, medicine and healthcare, scientific research (including space science), security systems and customs control, and more.

1.3. Radiation dosimetry

Radiation dosimetry is a branch of science that attempts to relate quantitatively specific measurements taken in a radiation field to the physical, chemical, and/or biological changes that radiation causes in target objects. Dosimetry is necessary for:

- Quantitative assessment of the frequency of occurrence of various biological changes depending on the amount of radiation received (dose–effect relationship);
- Comparison of various radiation experiments;
- Monitoring radiation exposure of individuals; and
- Environmental monitoring.

The principal concepts, on which radiation dosimetry is based, were described and methods for their practical application were presented. Radiation dosimetry necessarily includes the measurement of radiation dose and absorbed dose.

By definition, irradiation can be measured operationally using “free-air” or “standard” ionization chambers. A free-air ionization chamber is not a practical instrument for measuring routine exposure. It is used primarily as a laboratory standard. For routine use, chambers can be constructed with walls made of a solid material with radiation response properties similar to those of air.

Determining the absorbed dose in irradiated tissues is one of the primary objectives of the medicinal dosimetry. Typically, X- and γ -ray doses in wall materials with a low- Z (where Z is the atomic number) will roughly correspond to doses in soft matter over a wide range of photon energies. This fact leads to the widespread use of plastics and other low- Z materials for γ -dosimeter wall materials. To measure the dose/dose rate from a charged particle beam, it is necessary to measure the current flowing through a thin-walled ionization chamber located at different depths in the water target exposed to the beam. In this case, the dose rate is proportional to the current.

Some gas ionization instruments, primarily used to measure γ -radiation dose, also show readings when irradiated with neutrons. This response is due to ionization occurring in the gas as a result of the collision of charged recoil nuclei with neutrons in the walls and gas. However, the magnitude of ionization will be proportional to the absorbed dose only if the incident neutrons satisfy the Bragg–Gray principle: if the gas is enclosed in a wall of the same atomic composition and if the wall satisfies the thickness conditions, then the energy absorbed per unit mass of the gas is equal to the number of ion pairs formed there, multiplied by the average energy required to form an ion pair and divided by the mass of the gas. The carbon–carbon dioxide C–CO₂ chamber can be used for neutron dosimetry if its response has been experimentally calibrated as a function of neutron energy.

Let us briefly describe other important dosimetric quantities and concepts:

- To determine the equivalent dose of a neutral (neutrons or γ -ray) radiation, in addition to the absorbed dose, it is also necessary to know the LET (Linear Energy Transfer) of the incident or recoil charged particles formed during the irradiation.
- The quantity associated with dose from an indirect ionizing radiation by neutrons or photons is the initial kinetic energy of all charged particles released per unit mass. This quantity, which has the dimensions of absorbed dose, is called KERMA (Kinetic Energy Released per unit Mass).
- A particle- or photon-interaction within a small volume of tissue is an energy absorption event. The energy absorbed from the incident particle and all secondary electrons in the volume is called the imparted energy ε . Due to the statistical nature of radiation interactions, ε is a stochastic quantity. The imparted SE (Specific Energy) in a volume of mass m is defined as $z=\varepsilon/m$.
- The LE (Lineal Energy) γ is defined as the ratio of the energy ε imparted from a single event in a small volume and the mean length x of isotropic chords through the volume: $\gamma=\varepsilon/x$.
- The absorbed dose is an average value and therefore does not reflect the statistical nature of the energy distribution of ionizing radiation in matter. These aspects are particularly important when

considering the dose in small regions of the irradiated target, such as cell nuclei or other cellular components. MD (MicroDosimetry) studies these phenomena.

- Procedures have been developed for assessing effective and equivalent doses from internal sources of radionuclides that can enter the body through the inhalation, ingestion, wounds, or other means. ID (Internal Dosimetry) focuses on determining the equivalent dose received by various organs and the effective dose resulting from the ingestion of radioactive materials.

Monte Carlo radiation transport modeling is considered the gold standard in predicting radiation fields. This method uses computer simulation to model the paths and interactions of primary and secondary radiations from an initiating event through one or more media (simulated, shielding, detector materials, etc.). Properties of interacting particles can be monitored to estimate physical parameters of interest, for example, dose or KERMA. Many Monte Carlo codes are used for radiation transport modeling, reflecting the preferences of developers: high-energy physics, reactor core reactivity, medical physics applications, etc.

The earliest review [5] gave a brief description of the applications of boron isotopes nuclear properties, including neutron counters and energy sensors for neutron detectors. The structures of neutron sensor devices based on boron-containing materials were also described in a later review [6] devoted to boron isotope effects in solid materials.

Neutron-fluence nanosensors are nanotech-integrated monitoring tools that are helpful in reducing environmental risks. Concern over the consequences of harsh radionuclide pollution has resulted in an increasing demand for suitable means of monitoring neutron radiation sources: radioactive pollutants generated directly or indirectly, as a result of nuclear waste, influence different substances (water, gases, metals, etc.) used in nuclear power plants or places existing near radioactive materials. The development of a class of neutron-sensor materials has provided devices with enhanced selectivity and sensitivity for neutron radiation by a number of substances from harsh sites. On the other hand, state-of-the-art nanotechnology offers multiple benefits for neutron radiation-sensing applications: the ability to incorporate nano-sized radiation indicators into widely used materials such as paints, coatings, and ceramics to create nanocomposite materials; the development of ultralow-power, flexible detection systems that can be portable or embedded in clothing or other systems; and so on. Earlier data on boron-based neutron detectors summarized review [7].

Here, based on the concept of using boron isotopes in neutron sensors and detectors, a literature review is presented on their operating principles, design, and characteristics.

2. Boron-containing gases

A most common boron-based slow neutron detectors (Figure 1) consist of a proportional counter filled with a boron-containing gas, typically boron trifluoride BF_3 . To increase sensitivity, the boron is usually enriched in ^{10}B above its natural isotopic abundance of 19.7%.



Figure 1. Common slow neutron detectors containing counter filled with BF_3 gas [3].

In the idealized case, when the tube dimensions are too large compared with the reaction products ranges, response pulse heights at the E values of 2.31 and 2.79 MeV should be observed with peak areas in the ratio 96:4 (Figure 2-1). With practical sizes, however, a significant number of Li nuclei and α -particles enter the tube wall. Since these two reaction products separate “back-to-back” to conserve momentum, when Li strikes the wall the α -particle is directed away. This “wall effect” introduces continua to the left of the mentioned peaks (Figure 2-2). One continuum takes off from the peak at 2.31 MeV and is approximately flat down to 1.47 MeV. Over this interval, the total energy 1.47 MeV of the α -particle is absorbed in the gas while only part of the energy of the Li nucleus is absorbed there. Below 1.47 MeV, the spectrum again drops and is approximately flat down to the energy 0.84 MeV of the Li recoil. Pulses occur when the Li nucleus stops in the gas and the α -particle enters the wall. A similar continuum occurs below the smaller peak at 2.79 MeV. In other designs, boron compounds are used to line the interior walls of the tube filled with another gas, more suitable for counting.

The energy released in the $^{10}\text{B}(\text{n},\alpha)^7\text{Li}$ nuclear reactions results in a relatively large pulse amplitude, allowing the BF_3 proportional counter to discriminate neutron interactions from associated γ -reactions, which are usually present with neutrons and produce secondary electrons that ionize the gas. Compared

with the neutron reaction products, electrons produced by the photons are sparsely ionizing and give much smaller pulses. Amplitude discrimination can be used to eliminate these counts as well as electronic noise if the γ -fluence rate is not too large. In intense γ -fields, however, the pileup of multiple pulses from photons can become a problem.

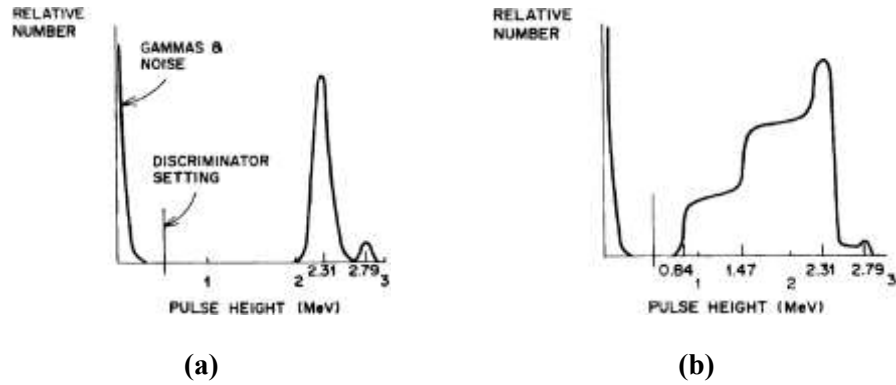


Figure 2. Pulse-height spectra from (a) idealized thermal-neutron large BF_3 tube, in which reaction products are completely absorbed in the gas, and (b) BF_3 tube showing wall effects [1].

When using BF_3 detectors as long counters with constant efficiency over a wide energy range, their tubes are often surrounded by moderating materials (usually polyethylene and cadmium) to increase sensitivity to fast neutrons (Figure 3).

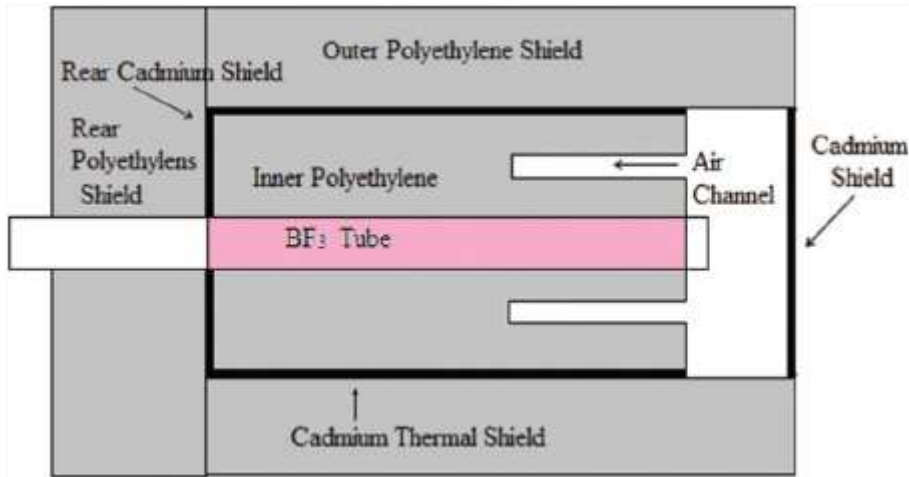


Figure 3. Schematic of BF_3 detectors with tube surrounded by polyethylene and cadmium shields [3].

The reaction $^3\text{He}(n,p)$ has the highest cross section of the above three usually used for slow-neutrons detection. Like the BF_3 tube, the ^3He proportional counter exhibits wall effects. However, ^3He is a better counter gas and can be operated at higher pressures with better detection efficiency. On the

other hand, because of the low E , though, γ -discrimination is worse. As for the ${}^6\text{Li}(n,\alpha)$ reaction, compared with ${}^{10}\text{B}(n,\alpha)$ one, it has a higher E and, potentially, better γ -ray discrimination, but lower cross section and, therefore, less sensitivity. Besides, the isotope ${}^6\text{Li}$ is only 7.42% abundant in nature. Note in this regard that, lithium scintillators are also used for slow-neutron detection. They can be made large compared with the ranges of the reaction products, so that the spectra are free of wall effects. However, the scintillation efficiency is then comparable for electrons and heavy charged particles, and so γ -ray discrimination is much poorer than with BF_3 gas.

Boron trifluoride BF_3 gas detectors can be used for moderated neutron as well. A detector of cylindrical long counter type is constructed to give nearly the same response from a neutron of any energy from about 10 keV to 5 MeV. It contains a BF_3 tube surrounded by an inner paraffin moderator. The instrument is sensitive to neutrons incident from the certain direction. Others either reflected or thermalized by the outer paraffin jacket and then absorbed in the boron-rich (usually, boron oxide B_2O_3) layer. Note that, such counters do not measure neutron spectra: the ${}^3\text{He}(n,p)$ and ${}^6\text{Li}(n,\alpha)$ nuclear reactions remain the only ones of major importance for neutron spectrometry.

Despite the lower achievable efficiency, toxicity, and corrosive activity, neutron detectors filled with boron trifluoride BF_3 are still used. Less abundant ${}^3\text{He}$ has failed to become an affordable alternative: the list of suitable neutron converters is quite short, and the serious shortage of ${}^3\text{He}$ requires the evaluation of all possibilities, including BF_3 [8]. The re-examination of BF_3 is also motivated by the modernization of neutron ToF (Time-of-Flight) spectrometers, which require large active areas. Discussions concluded that BF_3 could be replaced ${}^3\text{He}$ more or less directly, with certain limitations. Position-sensitive neutron detectors filled with BF_3 are a plausible option for replacing ${}^3\text{He}$ in large-area detection systems for ToF instruments. Due to their smaller conversion cross-section and reduced maximum pressure, they are best suited for the detection of cold neutrons.

A recent paper [9] reviews the physical principles of operation and characteristics of thermal neutron detectors filled with BF_3 gas. It is mentioned that although gas-filled radiation detectors are the earliest type of nuclear radiation detectors, their use persists due to their versatile characteristics, such as low cost, simple design and manufacture, ease of operation, long service life, etc. These detectors are still used in real-time applications, such as delayed neutron activity monitoring in pressurized heavy water nuclear reactors to detect faulty fuel, nuclear waste monitoring and special nuclear material detection systems.

3. Boron modifications

Crystalline semiconductor boron was used in neutron thermometers [10]. Such neutron sensors had advantages over more traditional gas-filled ones: neutron detectors built from boron-rich semiconductors could be particularly effective due to the easily detectable reaction products of neutrons with the ^{10}B nucleus. A boron-based neutron detector was first described in [11]. A pair of thermistors were matched for their identical semiconductor, but different nuclear properties: one thermistor was made of ^{10}B , and the other of ^{11}B . Both isotopes are stable, but when exposed to thermal neutrons, only the ^{10}B nucleus underwent a transformation. The significant amount of released average energy (2.79 MeV) led to the conversion of the signal into an electrical one. The formation of the rectifying contact on the ^{10}B sample allowed its application in a different type of solid-state neutron detector [12]. Its principle of operation is based on the generation charge carriers due to absorbing ^4_2He , that is, α -particle, ejected in the process of neutron interaction with boron.

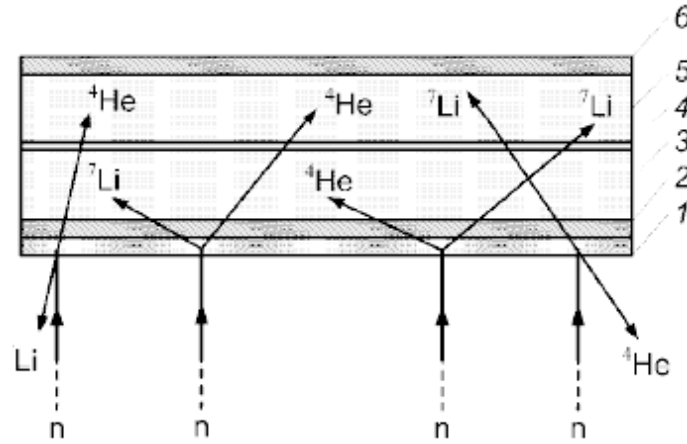


Figure 4. ^{10}B 2D-detector concept: (1) ^{10}B -layer, (2) Al-layer, (3) first sensitive gas gap, (4) W/Re-wires, (5) second sensitive gas gap, and (6) fiber glass layer [13].

A hybrid position-sensitive neutron detector with a ^{10}B active layer and a proportional counter chamber filled with a 25% CO_2 +Ar gas mixture (Figure 4) was investigated in [13]. The detector is used at a neutron source located on a linear accelerator. Registration of two pairs of pulse amplitudes generated in two gas gaps by ^4He and ^7Li nuclei between the anode and two cathodes allows one to determine the X and Y coordinates of neutrons and perform ToF measurements. A significant difference in the pulse amplitude spectra for slow and fast (with energy of several MeV) neutrons was observed. In experiments with the ^{10}B detector, it was found that: (1) Pulse amplitudes depend on the neutron energy, and (2) Position of the maximum in the pulse amplitude spectrum varies monotonically depending on the

maximum neutron energy. This 2D detector consists of ^{10}B , Al, sensitive gas gap, glass fiber layers, and WRe wires as well.

As is known, the two stable isotopes of boron, ^{10}B and ^{11}B , differ significantly in their neutron capture cross sections: for thermal neutrons, they are 3837 and 5 b, respectively. The high neutron capture cross section of ^{10}B nuclei, combined with its monotonic dependence on neutron energy, makes structural modifications of boron (as well as compounds and composites with high boron content) very attractive for the development of efficient neutron detectors. The concept of neutron detectors and sensors based on boron isotopes was presented [14] through an analysis of their operating principles, design, and characteristics. In particular, for boron-based neutron detectors the following were considered:

- Types: gas-filled; scintillation; solid-state; multilayer; combined, e.g. with gas-electron-multiplier technology; etc.
- Applications: monitoring of nuclear reactors, accelerators, and environmental neutron sources, including cosmic rays; radiation safety and nuclear security; neutron imaging, diffraction and spectroscopy to study the shape of objects and the structure and dynamics of materials; medicine, e.g. BNCT (Boron Neutron Capture Therapy); etc.
- Advantages: high neutron absorption cross-section, especially thermal; relatively low cost and availability of boron-containing materials; compact and robust solid-state detectors; potential for high detection efficiency; combination with other technologies to enhance performance; etc.
- Challenges: γ -rays discrimination, as they can interfere with neutron detection; pile-up effects in high-flux environments, potentially affecting neutron-counting accuracy; etc.

In the review [15], along with the basic information on the properties of borophene (the most promising and lightweight 2D-dimensional material), a summary of its application in biosensors and bioimaging is provided, and it is demonstrated that borophene-based nanosensors for biological molecules can find therapeutic applications, in particular, as a drug delivery platform used in BNCT.

A vertical borophene–graphene heterostructure formed by epitaxial growth of borophene (with a crystal structure closely matching that of α' -boron sheet) on multilayer graphene on copper substrate as a photodetector exhibits [16] excellent broadband photoresponse from UV (UltraViolet) 255 nm to IR (InfraRed) 940 nm, with enhanced sensitivity compared to pristine borophene or graphene-based photodetectors. A self-driven NIRPD (Near InfraRed PhotoDetector) based on multilayer α' -4H-borophene/GaAs heterojunction was fabricated [17].

Dispute traditional photoconductive detectors, it transfers the incident light energy into photocurrent realizing practically zero power dissipation. The borophene/GaAs NIRPD has high-level responsivity and specific detectivity, fast response/recovery time of ~ 100 ms, which are superior to some other photodetectors based on typical 2D materials such as boron sheet, graphene, and molybdenum diselenide MoSe_2 .

4. Boron-rich compounds

Single crystals of boron phosphide BP were studied in [18] for the development of refractory electrical devices such as solid-state neutron detectors using a large cross section of the ^{10}B isotope. The isotopic composition of the 200–300 μm thick wafers used was $(^{10}\text{BP})_{0.95}({}^{11}\text{BP})_{0.05}$. They were grown on silicon substrates by thermal decomposition of 1% $^{10}\text{B}_2\text{H}_6$ –5% PH_3 – H_2 gas.

In the neutron detector [19] based on semi-insulating boron-rich semiconductor crystal with an external bias voltage, a neutron interaction with ^{10}B nucleus produces ${}^4_2\text{He}$ and ${}^7_3\text{Li}$ nuclei. Both are rapidly stopped (within ~ 10 μm) in the semiconductor, exciting of electron–hole pairs. These free charges drift in the electric field, generating a measurable current pulse.

The materials that can be used include boron phosphide BP, selenide B_2Se_3 , sulfide B_2S_3 , and other wide-bandgap semiconductor boron compounds with relatively low melting temperatures, which facilitates their growth, for example, by CVD (Chemical Vapor Deposition) on silicon.

Boron carbide B_4C and hexagonal boron nitride h-BN are the two most commonly used semiconductor boron compounds used as base materials for neutron detectors. Therefore, we will consider them separately below.

4.1. Boron carbide

The idea of creating a boron carbide neutron flux fluence sensor was emerged [20] based on its unique complex of physical properties. The principle of this sensor is based on changing the electrical resistance of a B_4C sample due to lithium impurity atoms formed in the $^{10}\text{B}(\text{n},\alpha){}^7\text{Li}$ nuclear reaction. Thin films of B_4C are of particular interest for this purpose. B_4C films were prepared by laser deposition, using boron enriched in the isotope ^{10}B to increase the yield of the $^{10}\text{B}(\text{n},\alpha){}^7\text{Li}$ nuclear reaction. The films were deposited on sapphire substrates. Depending on the deposition conditions, the films had an amorphous, polycrystalline, or oriented structure.

The film thickness was tenths of μm . In the first series of experiments, B_4C films were irradiated with a thermal neutron flux in a dry reactor channel, while in the second one, they were placed in cadmium ampoules during irradiation to protect them from thermal neutrons. The dependences of the change in relative resistivity of oriented B_4C films on thermal and fast neutron fluence were obtained. Over the range of fluences achieved, this dependence was linear, with the effect of fast neutron irradiation being significantly greater than that of thermal neutrons.

Thermal neutron irradiation triggers three processes: (1) Formation of lithium impurity atoms in the B_4C semiconductor; (2) Formation of defects in the B_4C crystal lattice due to internal bombardment of atoms by α -particles; and (3) Formation of defects due to the residual fast neutron background. Since Li atoms in B_4C are donor impurities with low ionization energies, their appearance should decrease the film's electrical resistance. In turn, the formation of radiation defects in the film should increase the film's electrical resistance. Since it increases experimentally with increasing fluence, the main effect is likely related to the formation of defects.

Under fast neutron irradiation, the influence of donor impurities can be completely neglected. The increase in electrical resistance in this case can then be qualitatively explained by the appearance of defects in the B_4C crystal lattice. Thus, the observed increase in electrical resistance in both cases can be qualitatively explained by the appearance of defects in the B_4C crystal lattice (under both thermal and fast neutron irradiation).

Just the linear dependence of the relative change in resistivity on neutron flux fluence can be used to create a thin-film neutron fluence sensor. Since the observed changes are quite large (and reliably measurable), such a sensor could be used to create a simple device for measuring neutron flux intensity over a wide fluence range.

A proposed [21] boron carbidebased thermoelectric device for detecting thermal neutron fluxes (Figure 5) exploits, on the one hand, the very high melting point and radiation resistance of boron carbides, which made them suitable for use in aggressive environments, such as nuclear reactors, and, on the other hand, the anomalously large Seebeck coefficient of boron carbides, offering a relatively sensitive detector of localized heating that follows neutron absorption by the ^{10}B nucleus.

The possibility of developing boron carbide based neutron detectors on was also considered in [22]. Since ^{10}B is an excellent absorber of thermal neutrons, they cannot penetrate (to a depth of more than ~ 1 mm) into the ^{10}B -enriched material before absorption. Upon absorption of a neutron, ^{10}B decays into ^7_3Li and ^4_2He , thereby heating the material in the immediate vicinity of the neutron absorption site. In

this case, a temperature difference is established between the faces of the boron carbide sample. This difference can be controlled using the large Seebeck effect of boron carbide. In general, boron carbides can serve as simple, small, and robust (since the damage from neutron radiation caused by the decay of the ^{10}B isotope in icosahedral boron-rich solids is minimized due to the self-healing property of such structures) neutron detectors.

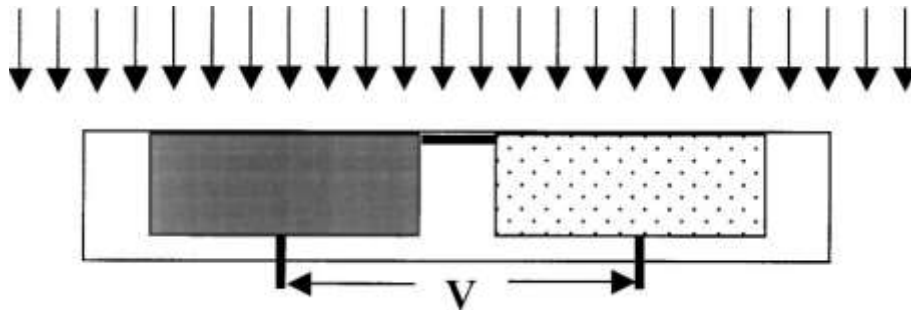


Figure 5. Boron carbide based thermoelectric detector of thermal neutrons: impinging arrows – neutron flux; boxes shaded darkly and filled with dots – detector’s active part made of boron carbide isotopically enriched in ^{10}B and ^{11}B , respectively, and encased in neutron absorber; thick solid line –electrical link between front faces of two boroncarbide parts; and two external electrical leads from their back faces to measure net Seebeck emf [21].

In the face of a shortage of ^3He , the most common isotope used in neutron detection, efforts are being made to develop viable neutron detection methods using alternative isotopes such as ^6Li , ^{10}B , and ^{157}Gd , which also have high neutron capture cross sections. In particular, technologies such as GEMs (Gas Electron Multipliers) have been used in combination with neutron converters. A prototype detector consisting of a double GEM stack with an aluminum cathode coated with a $^{10}\text{B}_4\text{C}$ layer was presented in [23]. Thermal neutrons are absorbed by boron via the $^{10}\text{B}(n,\alpha)^7\text{Li}$ reaction, and helium and lithium ionize the Ar- CO_2 gas (90:10) of the active volume of the detector, which is in open flow. After undergoing two-stage multiplications in the GEM, electrons are captured in readout strips. Resistive networks, using only 4 channels for 4 signals at each (X and Y) end, perform the strip readings. The fifth channel is then used to collect the fraction of electrons from the multiplication process that reach the bottom of the GEM’s lower electrode.

Currently, neutron detection is primarily based on ^3He gas detectors, but its shortage and the constant modernization of neutron facilities require new devices to conduct experiments with maximum efficiency. Such new detector based on a GEM in combination with multiple boron layers was presented in [24]. It combines the features of GEM technology with the properties of boron as a neutron converter, and the device is designed to support high neutron fluxes with high detection efficiency. The detector

demonstrated good response to (epi)thermal neutrons, achieving a detection efficiency of 16% at 1.8 Å (25 meV). High efficiency (even increased by additional GEM boron foils) and good time resolution make the detector a unique device for neutron detection methods. In particular, its use can easily be envisaged in methods involving neutron transmission measurements, which require high fluxes incident on the detectors, with the added benefit of 2D resolution thanks to the compacted anode. Embedding a single boron layer within the GEM detector block enables detection of thermal neutrons. Detection efficiency can thus be increased by depositing $^{10}\text{B}_4\text{C}$ layers directly on both sides of the GEM foil, creating a BGEM (Boron–GEM) foil, which exhibits a linear count rate dependence solely on the number of added double layers. Based on this concept, an improved medium-sized BGEM detector was designed and implemented to achieve an efficiency of approximately 20% for thermal neutrons at a sustained count rate of ~ 10 MHz/mm².

Solid-state real-time neutron detectors were also fabricated [25] from various semiconductor boron–carbon alloys produced by PECVD (Plasma-Enhanced CVD). Single neutrons were detected, and γ -induced signals were found to be negligible. Closo-1,2-dicarbadoecaborane (ortho-carborane) was used as the source gas to fabricate boron–carbon alloys with the natural isotopic abundance of ^{10}B . Devices fabricated from thicker layers of boron-carbon alloy enriched in ^{10}B resulted in increased detection efficiency. Active diodes could utilize their inherent μm -scale spatial resolution, expanding the range of applications.

Neutron detection with high total efficiency and higher resolution in kinetic energy, time, and/or position in real space is fundamental to the advancement of fields such as nuclear medicine, high-energy physics, special nuclear materials non-proliferation, astrophysics, structural biology and chemistry, magnetism, and nuclear energy. Smart indirect conversion geometries, interaction/transport calculations, and modern silicon and gallium arsenide processing techniques enable the creation of medium- and high-efficiency neutron detectors thanks to low defect concentrations, optimized reaction product ranges, improved effective omnidirectional cross sections, and reduced electron–hole pair recombination at sharper physical and electronically engineered interfaces. In turn, semiconductors with high neutron absorption cross sections and unique conversion mechanisms capable of achieving very high total efficiency are gaining increasing acceptance, despite the relative immaturity of their growth, lithographic processing, and understanding of their electronic structure.

The review [26] devoted to such achievements and problems in the geometry of charged particle devices, materials, and associated mechanisms of direct and indirect transduction of thermal neutrons

into fast ones in the context of their applications. In particular, the reactions and interactions arising from the capture and scattering of incident neutrons from ^{10}B and ^1H in amorphous hydrogenated boron carbide $a\text{-B}_5\text{C:H}_x$ (Figure 6) were considered.

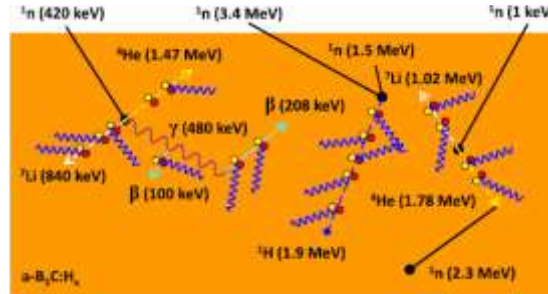


Figure 6. Reactions and interactions encountered from capture and scattering of incident neutrons with ^{10}B and ^1H in amorphous hydrogenated boron carbide $a\text{-B}_5\text{C:H}_x$: dashed lines and squiggles, respectively, show producing of electron–hole pairs through ionizing energy loss and corresponding energy given up to phonons [26].

4.2. Boron nitride

For neutron dosimetry, ceramic boron nitride h-BN is a good converter due to its high boron concentration and smooth surface. For this purpose, a plastic track detector [27] combined with a BN converter using (n,α) reactions was used. The efficiency was $1.0 \cdot 10^{-3}$ pits/n, which corresponds to a sensitivity of $9.6 \cdot 10^2$ mSv·pits/mm²; the linear response was in the range from 0.035 to 0.700 mSv; and the minimum detectable equivalent dose was estimated to be approximately 0.005 mSv. BNCT uses high-intensity neutron radiation: up to 10^9 cm⁻²·s⁻¹. To estimate the prescribed dose, it is important to separately record similar thermal neutron fluxes and the accompanying γ -doses. Later, for the BNCT it was proposed a thermal neutron shielded GRD (Glass-Rod Dosimeter) [28]. A BN thermal neutron converter was also developed to evaluate the neutron flux.

Epitaxial layers of h-BN synthesized by the MOCVD (Metal Organic Chemical Vapor Deposition) method were obtained [29] for application in neutron sensors. The thermal neutron absorption coefficient and absorption length of h-BN epitaxial layers with natural boron isotopic composition were approximately $0.0036 \mu\text{m}^{-1}$ and $277 \mu\text{m}$, respectively. To address partially the key requirement for long carrier lifetime and diffusion length for a solid state neutron detector, microstrip MSM (Metal–Semiconductor–Metal) detectors (Figure 7) were fabricated and tested. These detectors exhibited a good current response under continuous thermal neutron beam irradiation, corresponding to an effective conversion efficiency approaching ~80% for absorbed neutrons.

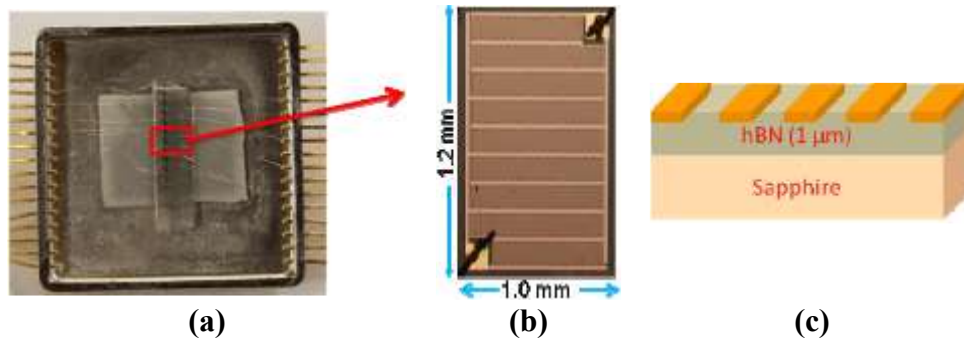


Figure 7. MSM h-BN based neutron detector in form of (a) package of (b) fabricated microstrips and (c) their schematic [29].

Due to the luminescent properties of GO (Graphene Oxide), which can be tuned by chemical processes, its ability to exhibit sufficient luminescence change upon exposure to γ - or neutron-radiation was investigated [30]. The mechanisms of radiation-chemical modifications and radiation-damage causing luminescence shifts in GO materials provided a fundamental basis for further development of radiation-sensitive detection architectures, as well as for the integration of h-BN with graphenebased devices to evaluate radiation-induced conductivity in nanoscale ones. The sensitivity of graphene transport properties to the presence of α -particles was demonstrated, and the successful integration of h-BN with graphene electrodes was discussed as a means of creating a basis for nanoscale radiation sensors (Figure 8).

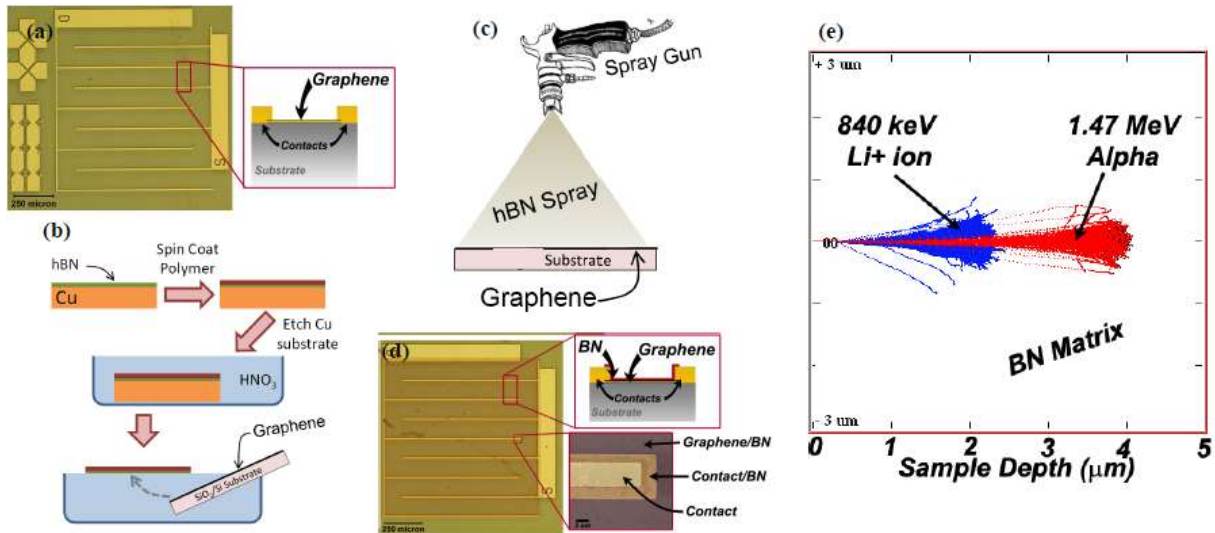


Figure 8. (a) Pristine graphene detector subsequently integrated with h-BN via (b) solution transfer or (c) spray deposition to form (d) graphene/h-BN detector (e) demonstrating that for initial neutron radiation induced α -particle penetration, ideal thickness of h-BN film is of $\sim 4\mu\text{m}$ [30].

According to the authors of [31], they reported the first successful demonstration of a direct-conversion semiconductor neutron detector with an overall thermal neutron detection efficiency of 4% and a charge collection efficiency of up to 83%, which was a μm -thick $\text{h-}^{10}\text{BN}$ epitaxial layer based (Figure 9a) and of the MSM type (Figure 9b). Such neutron detectors should offer all the advantages of semiconductor devices, including wafer-level processing, compact size, low weight, and the ability to integrate with other functional devices.

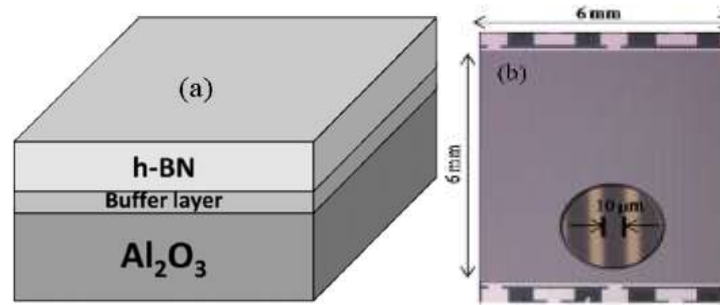


Figure 9. Direct-conversion semiconductor neutron detector: (a) schematic layer structure and (b) optical image of fabricated MSM detector incorporating 4.5 μm -thick h-BN epilayers [31].

In [32], processing and characterization of solid-state thermal neutron detectors based on h-BN were reported. These epitaxial h-BN layers with a natural ^{10}B content (19.9%) were grown by low-pressure CVD. Fully dry processing was used to fabricate detectors with MSM configuration. Produced detectors (Figure 10) exhibited intrinsic thermal neutron detection efficiencies of 0.86, 2.4, 3.15, and 4.71% for h-BN thicknesses of 2.5, 7.5, 10, and 15 μm , respectively. The measured efficiencies ($\geq 92\%$) are very close to the theoretical maximum efficiency values for the corresponding h-BN thicknesses for these detectors. This clearly demonstrates the scalability of h-BN thicknesses in detectors. An MSM detector based on 15 μm h-BN is expected to achieve an efficiency of 21.4% when using isotopically enriched (approximately 100% ^{10}B) h-BN instead of natural h-BN . These results demonstrate the feasibility of creating scalable, high-efficient thermal neutron detectors using h-BN .

In [33], the progress of h-BN -based solid-state neutron detectors using MSM technology (Figures 11 and 12) was briefly reviewed and it mentioned that an efficiency of 59% was achieved.

Since radioactive iodine vapor generated during nuclear fission can pose a significant risk to human health and the environment, effective monitoring of its leakage, capture, and storage is of great importance. In [34], a structurally and functionally integrated solid iodine vapor adsorbent based on metal-modified boron nitride BN aerogel was described. Such aerogels containing Cu/Ag nanoparticles

exhibit the high iodine vapor adsorption. To provide a basis for the development of multifunctional platforms based on metal-modified aerogels, an integrated iodine detection device was created. This device enables the detection of electrical properties of aerogels during iodine adsorption and lays the foundation for the development of BN aerogels for monitoring such radioactive contamination.

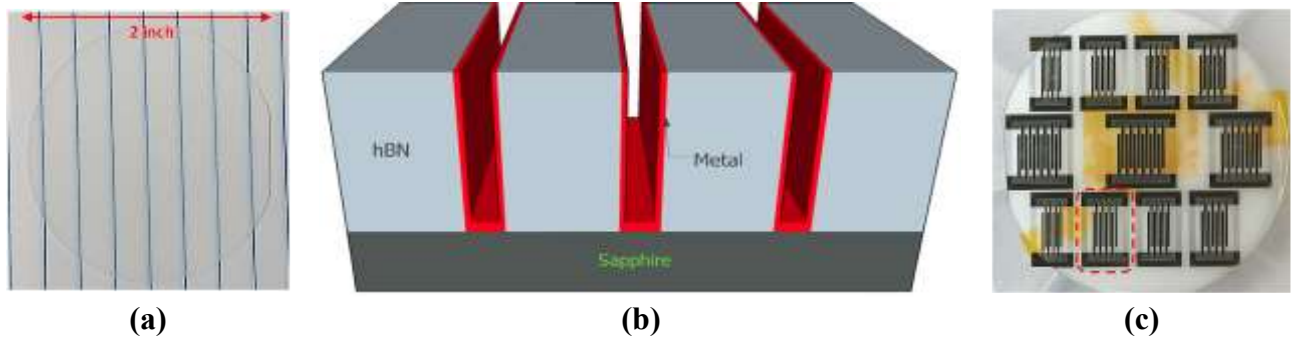


Figure 10. Solid-state h-BN based thermal neutron detector: (a) optical image of h-BN film on double side polished sapphire wafer placed on ruled paper, (b) schematic of h-BN MSM detector, and (c) optical image of detectors array fabricated using h-BN film [32].

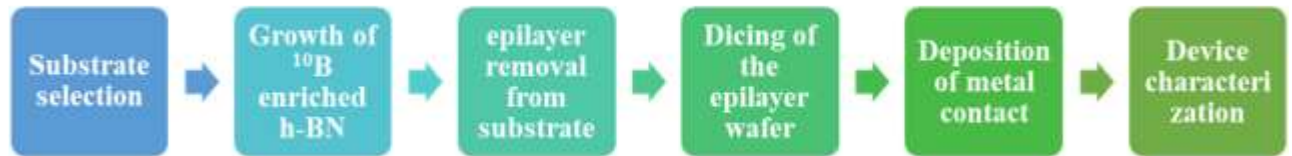


Figure 11. Schematic of h-BN detector fabrication process [33].

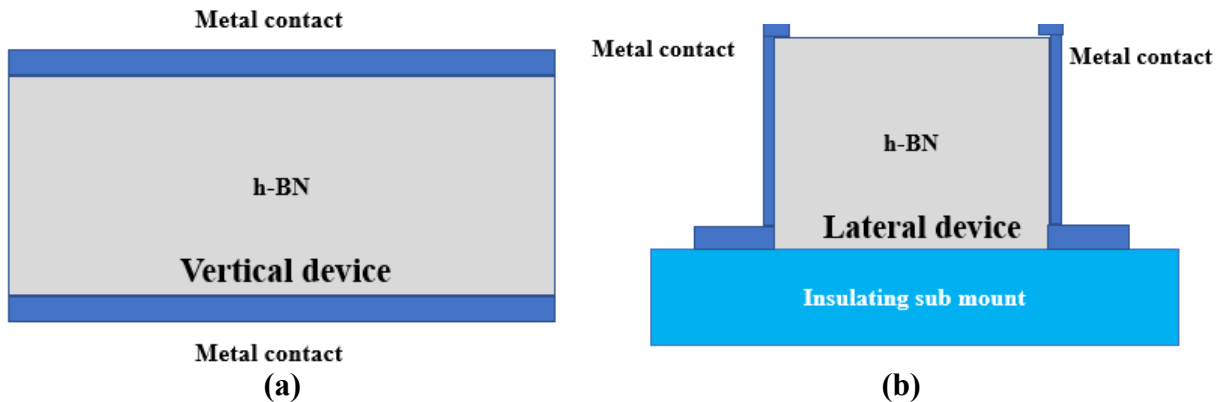


Figure 12. Cross-sectional schematic of (a) vertical and (b) lateral MSM neutron detectors [33].

Point defects in hexagonal boron nitride h-BN negatively affect neutron and deep-UV detectors by changing the properties of charge carriers. Several luminescent defects in h-BN show promise for quantum technologies. However, controlling PL (PhotoLuminescence) intensity and defect type remains a challenging task for the development of quantum emitters or sensors. In [35], the effect of helium ion and thermal neutron irradiation on the generation of vacancies and carbon-containing color centers in h-BN was studied. PL, Raman, and optically detected magnetic resonance measurements show that the defect density and type can be controlled by adjusting the irradiation doses. The number of carbon-containing color centers with a peak at ~ 580 nm can be directly increased in carbon-containing h-BN after such irradiations. Carbon-containing defects can also be created after annealing irradiated samples at 1300 K for 1 h. Interestingly, the optimal thermal neutron dose is $\sim 1 \cdot 10^{17}$ n/cm² for generating negatively charged spin defects of boron vacancies B_V^- in h-BN flakes of natural isotopic composition with improved spin properties. These results provide direct indications for the creation of B_V^- and carbon-related color centers and for understanding the effects of h-BN irradiation.

5. Boron-loaded materials

5.1. Boron-doped semiconductors

Among neutron sensor devices with increased selectivity and sensitivity, detectors based on thin semiconducting films doped with boron are naturally the best due to the special neutron capture properties of the isotope ^{10}B . In [36, 37], the key physical and technical characteristics of neutron detectors made of semiconductor materials enriched with ^{10}B were estimated: the thickness of the effective working layer is ~ 10 μm , the release rate of ^{10}B -n interaction products is $\sim 10^{15}$ cm⁻³·s⁻¹, the rate of generation of electron-hole pairs during neutron absorption is $\sim 10^{22}$ cm⁻³·s⁻¹, the rate of temperature increase is ~ 10 K·s⁻¹ and the average operating time of the device is $\sim 10^{-4}$ s.

Nanostructured films of germanium Ge and silicon Si doped with boron isotope ^{10}B are known to be the best materials for the preparation of highly effective and sustainable neutron-radiation sensors [38]. Boron atoms, originally shallow acceptors for Ge and Si, change their charge because of (n, α) nuclear reaction on ^{10}B stimulated by neutron irradiation bearing Li, which is a shallow donor for these semiconductors. Charge carrier concentration changes (a single captured neutron reverses a single charge) are easy to fix with the help of an electrical measuring instrument. This provides an opportunity to measure neutron fluence up to neutrons of very high density. These sensors rely on one or more sensing

mechanisms and produce a signal that indicates the nuclear/ionizing radiation value. For them it is also convenient to operate by so-called smart sensory systems.

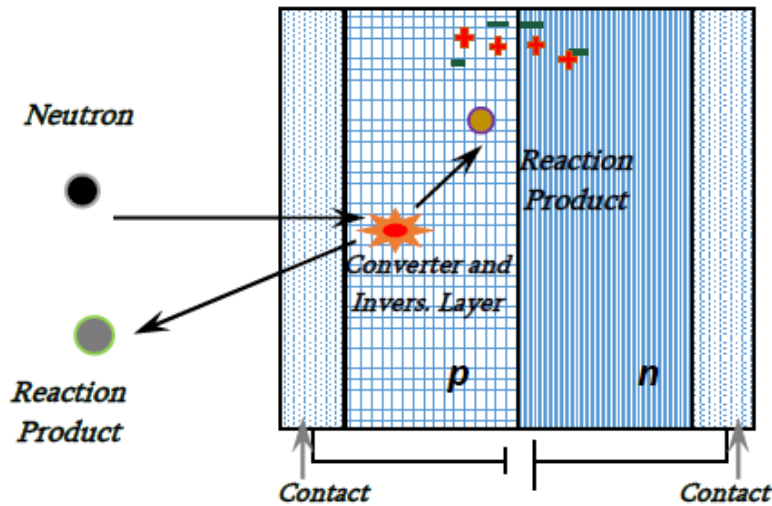


Figure 13. Schematic of ^{10}B -ion-implanted silicon diode with p–n junction for neutron detection [41].

A ^{10}B -ion-implanted silicon planar diode with a p–n junction for neutron detection (Figure 13) was created and studied [39, 40, 41]. The p-layer of the diode also serves as a neutron converter. ^{10}B nuclides with a high neutron capture cross section are used as converters. Neutrons are detected by registering the products ^4He and ^7Li of the $^{10}\text{B}(\text{n},\alpha)^7\text{Li}$ nuclear decay reaction. A diode with an inversion layer of hole conductivity created by implanting single-crystal n-Si with high-flux density ^{10}B ions. The absence of an independent converter in the planar detector simplify its manufacture and operation and reduces the cost. To determine the converter parameters, calculations of the ranges of ^4He and ^7Li ions and the spatial distribution of their ionization losses in silicon were performed. A specialized code was used to obtain a wider active ^{10}B layer, necessary for improving the sensor's efficiency. Simulations resulted in the selection of a sequential step-by-step ion implantation mode for ^{10}B ions with energies of 20, 35, 65, 80, and 100 keV. The ions source, current density, fluence, and implantation temperature were determined. Laboratory samples of ion-implanted diodes were obtained, and their current–voltage characteristics were determined.

An ion-implanted p–n junction planar diode for a neutron detector was fabricated by sequential ion implantation of a high-resistance single-crystal n-type silicon (100) surface with ^{10}B ions of varying energy and fluence [42]. The diode's inversion p-layer simultaneously serves as the detector's converter. A portable modular universal radiation detector was created based on this diode. The detector system

consisted of a detector, a preamplifier, a shaping amplifier, a comparator, a microprocessor unit, a keyboard, an LCD (Liquid Crystal Display), a bias generator, a battery-powered UPS (Uninterruptible Power Supply), and a battery. Software functions and libraries were developed to control the multicomponent assemblies of the detector system, as well as for statistical data analysis and interpretation of the results. Preliminary tests of the detector were carried out using α -particles (^{241}Am source) and neutrons (^{252}Cf source).

An ion-implanted silicon planar diode with a p–n junction for neutron detection was created and studied [43]. The p-layer of the diode also serves as a neutron converter. A batch of diodes was obtained by sequential ^{10}B ion implantation of single-crystal Si. Ohmic contacts made of Ti and Au were deposited on the p–n junction. The current–voltage characteristics of the diodes were studied. A prototype of the detector electronic system was developed and the noise level and filtering methods for the pulsed power supply were determined, as well as its effect on the sensitive analog parts of the detector, and various shielding methods for the analog unit. A modified functional prototype of the detector was also developed.

The acceptor removal process is the most detrimental effect observed in irradiated boron-doped silicon. This process is caused by a radiation-induced BCD (Boron-Containing Donor) defect with bistable properties, which are reflected in electrical measurements. The electronic properties of the BCD defect in its two different configurations, A and B, and the transformation kinetics were determined [44] from changes in the current–voltage characteristics in the temperature range from -30 to $+35^\circ\text{C}$. The changes in the depletion voltage are consistent with changes in the BCD defect concentration in the A configuration measured by the thermally stimulated current method. The A $\rightarrow$ B transformation occurs under nonequilibrium conditions when excess free carriers are injected into the device. The inverse B $\rightarrow$ A transformation occurs upon removal of nonequilibrium free carriers. Energy barriers of 0.36 and 0.94 eV were determined for the A $\rightarrow$ B and B $\rightarrow$ A configurational transformations, respectively. Determined transformation rates indicate that A $\rightarrow$ B and B $\rightarrow$ A defect transformations are accompanied by electron capture and electron emission, respectively. Such silicon detectors are extensively used for research in high-energy physics.

In order to achieve the goal of developing accurate and fast neutron sensors using boron isotopes, the following tasks for silicon-based devices were formulated [45]: (1) Development of the physical principles of operation of semiconductor sensitive nanoelements doped with boron isotopes and the basics of their manufacturing technology; (2) Using advanced technologies for producing elementary semiconductor sensor elements based on silicon enriched with boron isotopes and development of highly efficient

prototypes of nanosensors of improved designs; and (3) Study of the features of the technology for growing semiconductor thin films of silicon doped with boron isotopes and their properties, as well as research into the use of GFETs (Graphene Field-Effect Transistors) (Figure 14) as tools for increasing the sensitivity of measurements, which is due to the importance of the target for ultra-sensitive neutron detection.

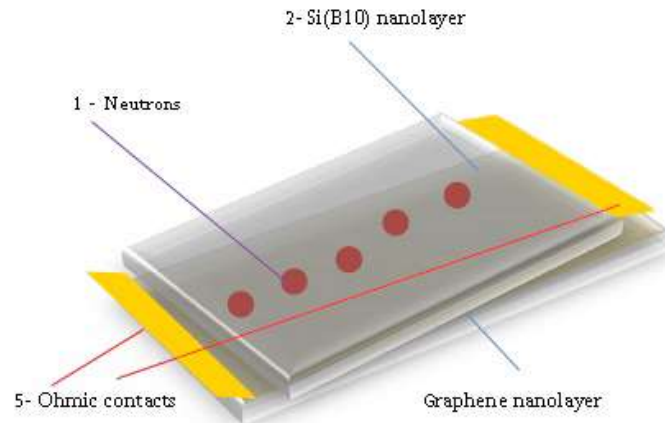


Figure 14. Schematic of silicon- ^{10}B -graphene sensitive element of neutron detectors [45].

5.2. Boron-containing composites

An old review [46] of dosimeters mentioned only three types of personal neutron dosimeters commonly used for radiation protection purposes: NTA (Neutron Type A) dosimeters, albedo TLDs (ThermoLuminescent Dosimeters), and fission track detectors. Insufficient energy sensitivity and response, fading, the use of radioactive materials, and some other limitations prevent any of these dosimeters, nor their subsequent modifications, from being satisfactory for general use in a wide range of radiation environments. To create a dosimeter capable of providing useful albedo neutron readings, it is necessary to remove or at least significantly reduce the number of incident thermal neutrons. This can be achieved by placing a thermal neutron-trapping material, such as plastic containing boron or cadmium, over a TLD.

Combinations of TLD and cadmium form common albedo neutron dosimeters (Figure 15a–f), in which the cadmium disk (Figure 15g) should be as large as possible to prevent incident thermal neutrons from entering the object (e.g. human body) near the TLD, where they have a high probability of being scattered and detected. Because thermal neutrons migrate long distances before being captured, the cadmium disk diameter should be ~ 10 cm. This is why the boron-doped plastic is preferable: the shielding effect of low-energy X- or γ -ray is significantly weaker, and only a single TLD is required. However,

boron-doped plastic has a draw back: the thickness required to stop all thermal neutrons is large compared to cadmium. To reduce it, the expensive isotope ^{10}B must be used.

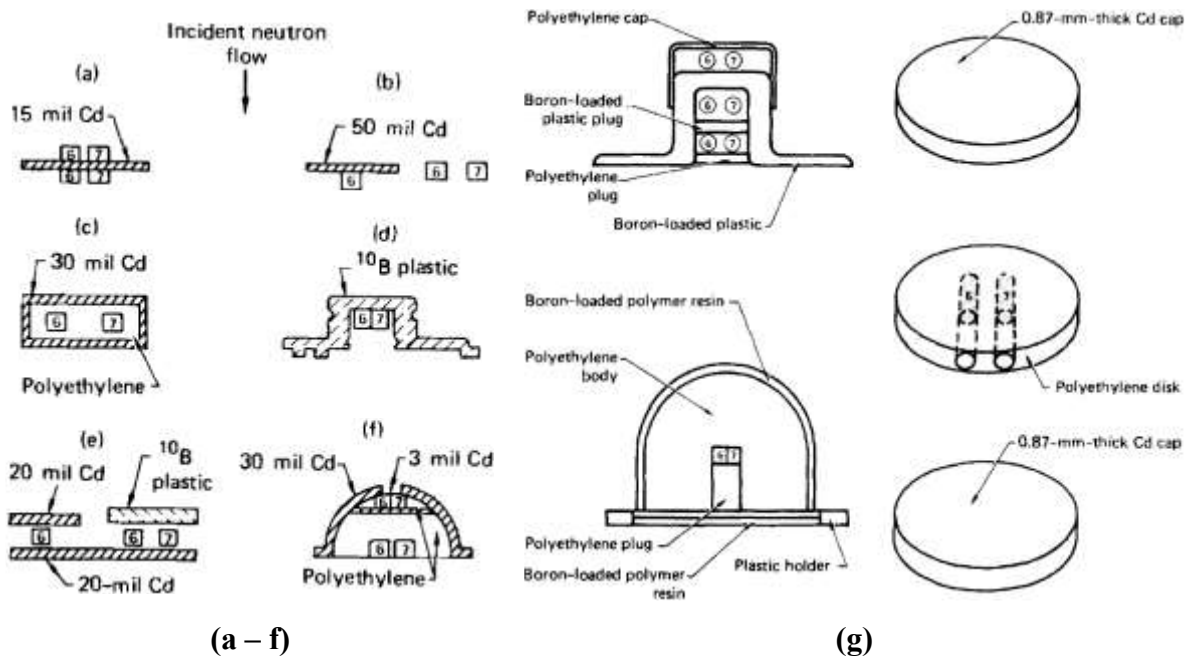


Figure 15. Common bedo dosimeters (a – f) designs and (g) cadmium disks; numbers 6 and 7 refer to ^6LiF and ^7LiF materials [46].

Another problem is that TLDs with boron and cadmium shielding give different readings when exposed to intermediate-energy neutrons. This is due to the different cross-sections of boron and cadmium near the thermal region. The magnitude of this difference provides information about the neutron energy spectrum. Unfortunately, it is too small for accurate assessment in the field.

A neutron dosimeter using spark track counting in a boron-doped thin (μm -scale) film was fabricated [47] on cellulose nitrate films loaded with a boron compound. After irradiation with thermal neutrons, the films were etched in aqueous solution of $\sim 10\%$ NaOH at $\sim 50^\circ\text{C}$ for ~ 1 h. Etch pits formed by $^{10}\text{B}(n,\alpha)^7\text{Li}$ nuclear reactions were punched twice at 600 V and then counted at a lower voltage of 500 V. The spark density ratio was of $\sim 10^{-4}$ at boron concentration of $\sim 1\%$.

In [48], highly sensitive, simple, and non-radioactive neutron dosimeters were manufactured in the form of plastic plates loaded with ortho-carborane, another boron compound. After irradiation with thermal neutrons, the plates were etched in aqueous KOH solution. Then, using optical microscope/automatic track counting system, the etch pits formed as a result of $^{10}\text{B}(n,\alpha)^7\text{Li}$ nuclear reactions were counted. At a constant etching time, the etch pit density is proportional to the flux of

irradiated thermal neutrons. The proportionality coefficient, called the “sensitivity”, was of $4.2 \cdot 10^{-4}$ for a plate containing ortho-carborane at a concentration of 0.5 wt.% with an etching time of 16 h. Taking into account background counts, it was found that this plate could measure a thermal neutron dose of 0.025 mSv. These plates are insensitive to visible, UV, X-ray, β -, and γ -radiation and are easy to handle because they combine the detector and converter.

An inorganic boron compound, lithium tetraborate $\text{Li}_2\text{B}_4\text{O}_7$, was also considered as an alternative [49] as a promising transducer for neutron dosimeters. The low reliability of sintered crystals as a dosimeter was overcome by creating them in the form of glass-ceramics $\text{Li}_2\text{B}_4\text{O}_7 + 5\% \text{SiO}_2 + 0.01\% \text{Pt}$ or thin deposited layers on LiF single crystal. Based on the information on the TSSE (Thermally Stimulated Exoelectron Emission) glow pattern of the duplicated structure, it is possible to measure the dose of each type of radiation separately in a mixed radiation field.

The boron-based thermal neutron detector (Figure 16) made in [50] contained four or more layers of natural boron (i.e. containing almost 20% of ^{10}B isotope) absorbing thermal neutrons. Thickness of a layer was $0.4\text{--}1.2 \text{ mg/cm}^2$. The layers were deposited on one or on both sides of metal surfaces used as contacts. Between the absorbing layers, there were gas-filled gaps 3–6 mm thick. Electric field of 100–200 V/cm was applied to them. When atoms of ^{10}B capture a thermal neutron, nuclear reaction occurs, as a result of which two heavy particles – α -particle and ^7Li ion – from the thin absorber layer are emitted in opposing sides. One of the two particles penetrates into gap and ionizes it. An impulse of electric current is created in the gas-filled gap actuated by the applied electric field. An electronic circuit registered the impulse. Detectors containing from 2 to 16 layers of natural boron with an efficiency of thermal neutron registration from 2.9 to 12.5% were made and tested.

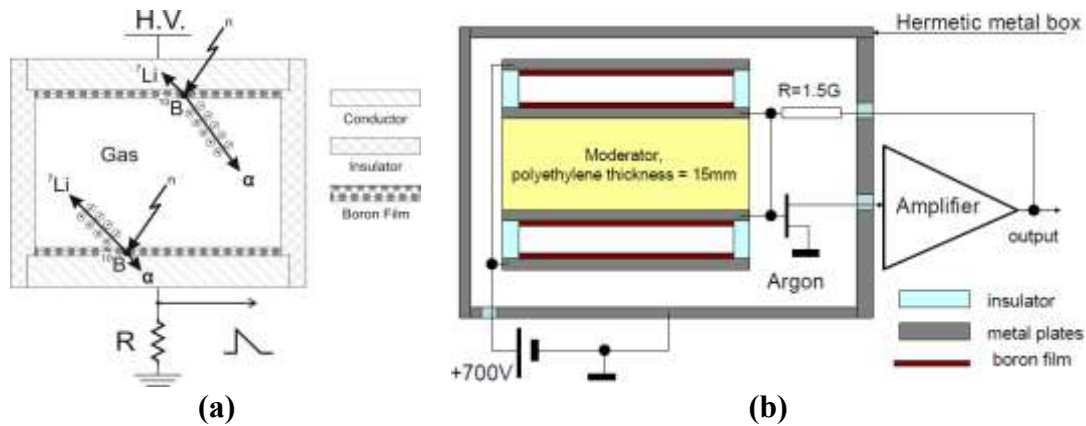


Figure 16. Boron based thermal neutron detectorschemes of **(a)** signal formation and **(b)** basic element connection [50].

In digital neutron imaging systems, the neutron scintillator screen is the limiting factor in spatial resolution and neutron capture efficiency should be improved to enhance their capabilities. Commonly used neutron scintillators are based on lithium fluoride ${}^6\text{LiF}$ or gadolinium oxysulfide ${}^{157}\text{Gd}_2\text{O}_2\text{S}$ neutron converters. Boron-based neutron scintillators were investigated [51] because ${}^{10}\text{B}$ has a neutron absorption cross section about 4-times larger than ${}^6\text{Li}$, less energetic decay products than ${}^6\text{Li}$ and ${}^{157}\text{Gd}$, and lower γ -ray sensitivity than ${}^{157}\text{Gd}$. All these factors indicate that, although boron-based neutron scintillators may produce less light than ${}^6\text{Li}$ -based screens, they can provide improved neutron statistics and spatial resolution.

A parametric study was conducted to determine the impact of various boron-based neutron converters, scintillator and converter particle sizes, converter-to-scintillator component ratios, substrate materials, and sensor design on image quality. The most efficient boron-based scintillator screens demonstrated improved neutron detection efficiency compared to a conventional lithium fluoride/zinc blende ${}^6\text{LiF}/\text{ZnS}$ scintillator, with 125 and 67% increases in thermal and epithermal neutrons detection efficiency, respectively. The spatial resolution of high-resolution boron-based scintillators was measured, and neutron tomography of a test object was successfully performed using boron-based screens demonstrating the highest spatial resolution. Boron-based scintillators can be utilized to enhance the performance of a digital neutron imaging system by reducing data acquisition time and improving neutron statistics.

The paper [52] reported progress in creating an organic glass scintillator with sensitivity to both thermal and fast neutrons, providing “triple” PSD (Pulse Shape Discrimination) by incorporating an aromatic molecule containing boron. The commercially available TDB (2-(p-Tolyl)-1,3,2-Dioxaborinane) can be easily synthesized in a single step using inexpensive materials and incorporated into the organic glass scintillator at 20 wt.% ${}^{10}\text{B}$. Furthermore, it was shown that TDB is easily scalable and can be incorporated into organic glass scintillator samples to produce the highest thermal neutron capture signal ever recorded.

Based on the results of in-depth studies using a crystal detector mounted on a photomultiplier tube enclosed in a lead chamber, it was concluded [53] that the boron-containing polymer phenylethenylboronic acid is an effective absorber of radiation, particularly X- and γ -rays, and neutrons. A computer program with powerful multichannel analyzer capabilities was used to obtain data during experimental geodetic surveys.

The development of radiation-shielding materials with high resistance to irradiation under reactor conditions is one of the pressing challenges of modern nuclear technology. UHMWPE (Ultra-High Molecular Weight PolyEthylene) is considered a promising matrix material due to its high hydrogen content, low density, and high chemical resistance. Composite samples based on it were fabricated and irradiated at various neutron fluences in a research reactor [54]. The results of measuring their neutron absorption capacity, bending strength, and chemical resistance before and after irradiation showed that boric acid H_3BO_3 makes the greatest contribution to increasing the neutron absorption coefficient, with the maximum effect observed at a filler content of 30%.

In general, UHMWPE-based composites containing boron and fillers with heavy elements (such as WC and PbO) demonstrate great potential as radiation-shielding materials. Tests have shown that UHMWPE composites with functional fillers combine different protective functions in a single material, which is traditionally achieved only with multilayer borated polymer–(lead, steel) systems or heavy monolithic shields. The hydrogen-rich UHMWPE matrix effectively slows down fast neutrons, while H_3BO_3 , and WC and PbO additives ensure thermal neutron capture and γ -radiation attenuation, respectively. The neutron absorption coefficient increases with H_3BO_3 content, demonstrating the ability to tailor protective properties to the required spectrum.

6. Calculation of neutron radiation fields

Intrinsic efficiencies of multi-layer ^{10}B thin-film detectors (Figure 17) were studied theoretically [55]. For multi-layer schemes based on an optimized single-layer film thickness, the practical efficiency is limited to about 42% for thermal neutrons. This is about half the efficiency of moderated ^3He detectors in commercial use for portal monitoring. The efficiency limitation is due to charged particle loss in the boron layers and substrates. The same loss mechanism will prevent all substrate-based boron detectors from ever reaching the intrinsic efficiencies of high-pressure ^3He tubes, independent of substrate geometry and material composition. Excellent n/γ discrimination was also been achieved using an ionization chamber. There are four possible scenarios of thermal-neutron detection using thin boron films on a substrate, depending on neutron incidence and film thickness. When the neutrons and the film are at opposite sides of the substrate, it is called the transmission mode. When the neutrons and the film are at the same side of the substrate, it is called the back-scattering mode. Both the transmission and the back-scattering modes can be further divided into two cases depending on the film thickness.

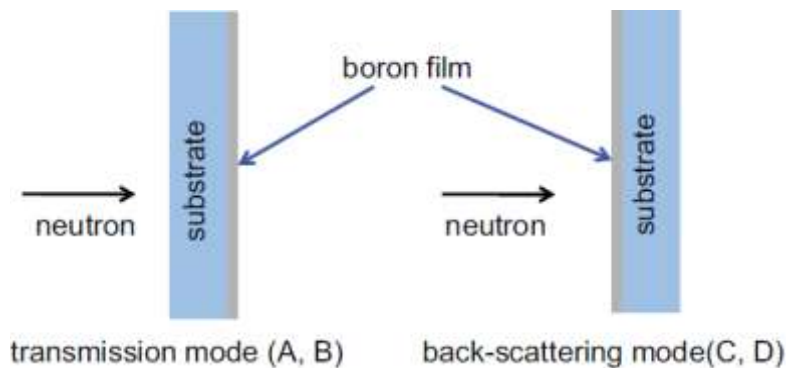


Figure 17. Four modes – A, B, C, and D – of thermal neutron detection by thin boron films depending on neutron incidence and film thickness [55].

SEUs (Single-Event Upsets) were measured in thermal neutron-irradiated microcontrollers with 65- and 130-nm node SRAMs (Static Random Access Memories) [56]. The proposed fault mechanism is charge deposition from the energetic byproducts of ^{10}B thermal neutron capture. Although elemental analysis confirmed the presence of ^{10}B in both microcontrollers, only the 65-nm node microcontroller exhibited a strong response to thermal neutrons. Monte Carlo simulations were conducted to investigate the effect of ^{11}B enrichment on thermal-neutron-induced SEUs in 65-nm node SRAM in the presence of boron in the p-type well, source, and drain, or tungsten plug. They show that $^{10}\text{B}(\text{n}, \alpha)^7\text{Li}$ nuclear reaction byproducts are capable of generating sufficient charge to disrupt 65-nm SRAM. The highest charge deposition from those byproducts occurs when natural boron is used to dope the p-type source and drain regions. Simulations also show that the disruption SEU cross-section becomes significant when ^{11}B -enriched boron is used as the dopant.

To study boron carbide B_4C as a nuclear reactor control rod material, the values of their important radiation interaction parameters such as MAC (Mass Attenuation Coefficient), LAC (Linear Attenuation Coefficient), HVL (Half-Value Layer), TVL (Tenth Value Layer), and MFP (Mean Free Path) were analyzed [57] using the PPD (Photon Protection and Dosimetry) software. In addition to B_4C , the following metallic cladding materials were considered: hafnium Hf, indium In, silver Ag, and cadmium Cd. The analyses were performed in the energy range of 1–15 MeV. At 1 MeV, the MAC values were 0.053 and 0.015 cm^2/g for Hf and B_4C , respectively; and at 15 MeV, the corresponding HVL values were 1 and 17 cm. Similarly, while the TVL value for Hf was approximately 5 cm, for B_4C it was determined to be 54 cm. The obtained results, especially for LAC, HVL, TVL, and MFP, are consistent with the literature data. The shielding and dosimetry parameters (effective atomic number Z_{eff} , electron density

N_{eff} , conductivity C_{eff} , etc.), as well as EAF (Energy Absorption Factor) and EBF (Exposure Accumulation Factor), for B_4C were investigated by a software allowing their simultaneous, quick, and accurate calculation in the desired energy ranges.

Neutron output assessment is important to ensure adequate patient dose. This requires effective QA (Quality Assurance) and QC (Quality Control) while maintaining measurement accuracy. The study [58] investigated the optimal activation measurement conditions for QA/QC in an AB-BNCT (Accelerator Based BNCT) system. Measurements were performed in a PMMA (MolyMethyl MethAcrylate) phantom using metal alloy foils. The relative expanded uncertainty in QA/QC activation measurements was $\sim 4.5\%$. The reusable 2D radiochromatic response-based detector [59] for dosimetric measurements in radiation therapy consists of a reusable 2D radiochromatic dosimeter in a cuboid container, connected to a flatbed scanner and data processor using a software package containing specialized functions for matching radiation and mechanical isocenters. This system was successfully applied for coincidence tests, confirming its suitability as a QA tool in radiation therapy.

To obtain an epithermal neutron field suitable for testing the performance of neutron detectors used in, a BSA (Beam Shaping Assembly) based on a deuterium–deuterium D–D neutron source was developed using Monte Carlo simulation and a multi-objective optimization algorithm [60]. First, the interaction of deuterium ions with a deuterated titanium target was calculated to determine the neutron source characteristics. Then, a multi-objective optimization of the BSA based on the D–D neutron source was performed to maximize the epithermal neutron flux and minimize fast neutron contamination and thermal neutron fraction. Finally, a 3D water phantom was used to evaluate the beam distribution characteristics. The results show that the epithermal neutron flux, fast neutron contamination, and thermal neutron fraction after optimization reached values that exceeded the expected ones. The neutron field at the BSA exit demonstrated good symmetry and directionality in its spatial distribution. The goal of this study was to provide reliable experimental conditions for the detectors development and calibration, as well providing ideas for miniaturizing BNCT devices.

Radiative thermal neutron capture (n, γ) can produce detectable, precise-energy nuclear recoils for detector calibration. An experiment to measure these twin products – the postcapture deexcitation gamma and postcapture NR (Nuclear Recoil) were proposed in [61]. A nucleus absorbs a low-energy ($\ll 0.01$ eV) neutron, which enters the nuclear system at the neutron separation energy ($\sim$ MeV), and very quickly ($\sim$ fs) the nucleus deexcites to its ground state, emitting a cascade of gammas. Each γ -emission causes a corresponding momentum change of the nucleus, though the cascade is so fast that all of the NR energy

comes in a single pulse for all detectors. To measure these events, it was proposed a minimal (simplest and cheapest possible version of) three detector experimental setup and modeled to estimate the postcapture γ -signal rate and the source-coincident backgrounds. The simulation geometry consisted of the detector stack, lead shielding, source cube, and world volume. Simulations show that with a 1 mCi californium neutron source, measurements with available detector technologies is possible in 26.1 g-days of exposure.

7. Obtaining methods

In nanostructured form, boron-rich materials exhibit properties that improve their radiation-protective properties. That's why, new technologies have been proposed for synthesizing nanocomposites with boron carbide B_4C and hexagonal boron nitride h-BN matrices.

To study the problem of developing new nanomaterials used as delivery agents for the boron ^{10}B isotope in BNCT, a mini-review was conducted [62] of: (1) Boron nanopowder compounds that are particularly promising for BNCT; (2) Magnetic nanocarriers of therapeutically active agents in general, the delivery of which can be controlled using an external magnetic field; and (3) Methods for synthesizing nanocomposites containing components of both types. Based on an analysis of the latest literature data, boron nitride and boron carbide nanopowders doped with ferromagnetic iron oxide nanoclusters are recommended for BNCT as effective delivery agents with good biocompatibility.

For the first time, composites of boron carbide–tungsten and hexagonal boron nitride–(iron, magnetite) [63] were obtained in the form of layered/“sandwich” structures of B_4C and W components and h-BN nanopowders coated/intercalated with magnetic nanoclusters of iron Fe or magnetite Fe_3O_4 . The study of their chemical/phase composition, structure/morphology and some other properties leads to the conclusion that the developed B_4C –W and h-BN–(Fe, Fe_3O_4) composites can be useful for solving important problems of boron-based neutron protection and BNCT, such as the attenuation of γ -radiation accompanying the absorption of neutrons by ^{10}B nuclei and the targeted delivery of ^{10}B nuclei as therapeutic agents of BNCT to tumor tissues using control by an external magnetic field, respectively.

It was shown both theoretically and experimentally that one of promising classes of neutrons shielding materials are composites of boron carbide with tungsten B_4C –W: inclusions of the tungsten phase containing heavy W atoms provide effective attenuation of secondary γ -radiation accompanying the absorption of primary neutrons by atoms of the boron isotope ^{10}B . Composites with “sandwich” and multilayer morphology – $W/B_4C/W$, $W/B_4C/W_2B_5$, $W_2B_5/B_4C/W_2B_5$, etc., in which layers of boron

carbide alternate with layers of metallic tungsten and/or tungsten pentaboride, were obtained and studied in [64]. Metallization of the surface of boron carbide crystals or grains with powder, plate, or coating of tungsten was carried out by SPS (Spark-Plasma Sintering), as well as standard thermal sintering. Structural and morphological analysis of the obtained samples using SEM (Scanning Electron Microscopy), phase analysis using XRD (X-Ray Diffraction) and analysis of the chemical composition using EDS (Energy-Dispersive Spectrometry) showed that transition layers of tungsten pentaboride W_2B_5 are formed at the B_4C –W interfaces, which ensures strong adhesion of the component layers.

Several chemical routes were proposed [65] for the synthesis of hexagonal boron nitride h-BN nanopowders doped with magnetic nanoclusters – ferromagnetic iron Fe or ferrimagnetic magnetite Fe_3O_4 . Nanocomposites obtained revealed magnetic properties rendering them useful for an application in BNCT for external magnetic field controlled delivery of neutron-capturing boron ^{10}B isotopes in target tumor cells.

8. Conclusions

In summary, the following aspects are considered for boron-based neutron detectors:

- Types: gas-filled, scintillator, solid-state, multilayer, combined (e.g., with gas electron multiplier technology);
- Applications: monitoring of nuclear reactors, accelerators, and environmental neutron sources (including cosmic rays), radiation safety and nuclear security, neutron imaging, diffraction, and spectroscopy (to study the shape of objects as well as the structure and dynamics of materials), medicine (e.g., BNCT);
- Advantages: high absorption cross section for neutrons (especially thermals), relatively low cost and availability of boron-containing materials, compact and reliable solid-state detectors, potential for high detection efficiency, combination with other technologies (to improve performance); and
- Challenges: γ -rays discrimination (as they can interfere with neutron detection), pile-up effects (in high-flux environments potentially affecting neutron counting accuracy).

It can be concluded that, despite the existing challenges, boron-based neutron detectors and sensors offer a versatile and effective way to detect and characterize neutrons in a wide range of applications.

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Laser-Plasma Mediated Thin-Film Development: Precision Engineering of Silicon-Carbon Nanosystems for Advanced Applications

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Abstract

Laser-plasma deposition (LPD) has emerged as a transformative physical vapor deposition technique for the development of advanced thin-film materials. This review provides a comprehensive analysis of LPD's unique capabilities in synthesizing and restructuring Silicon–Carbon (Si–C) nanosystems, with a particular focus on graphene-integrated silicon architectures. Unlike conventional thermal or chemical methods, LPD operates through a dynamic non-equilibrium process that inherently combines ablation, plasma formation, and surface restructuring. We examine how key parameters—laser wavelength, energy density, background gas, and substrate conditions—govern the phase composition, crystallinity, and interfacial properties of Si–C films. To conceptualize the intrinsic feedback between energy input and material response during LPD, we introduce the framework of self-control closed-loop (SCCL) dynamics. Furthermore, we employ the concept of dynamic fractal space (DFS) to model the topological evolution of Si–C systems under continuous energy enforcement. This integrated approach positions LPD not merely as a deposition tool, but as a *restructuring technology* capable of producing tailored nanoscale architectures—from highly ordered graphene on silicon to amorphous silicon carbide (a-SiC) coatings. We discuss resulting applications in high-efficiency hybrid photovoltaics, nanoelectronics, and spintronics, highlighting the role of LPD in enabling next-generation thin-film devices where precision, scalability, and multifunctionality are paramount.

Keywords: Laser-plasma deposition; Thin-film technology; Silicon-carbon systems; Graphene-silicon heterostructures; Dynamic fractal space; Self-control closed-loop systems; Nanoscale restructuring; Hybrid photovoltaics

1. Introduction: The Role of Laser-Plasma Processes in Modern Thin-Film Technology

Thin-film technology is the cornerstone of contemporary micro- and nano-electronics, photovoltaics, and functional coatings. The performance of these films is critically dependent on their microstructure, phase purity, and interfacial characteristics, which are, in turn, governed by the deposition technique [1]. Among physical vapor deposition methods, laser-plasma deposition (LPD)—encompassing pulsed laser deposition (PLD) and continuous-wave laser deposition (CWLD)—has gained prominence for its versatility, stoichiometric transfer capability, and suitability for synthesizing complex and metastable materials [2].

LPD's distinct advantage lies in its *inherently dynamic and far-from-equilibrium* nature. A focused laser beam ablates a target material, generating a dense plasma plume that expands toward a substrate where film growth occurs. This process integrates three fundamental stages—**destructuring** (ablation), **transport** (plasma expansion), and **restructuring** (condensation and nucleation)—within a single vacuum environment [3]. This review argues that it is precisely this integrated, energy-driven restructuring capability that makes LPD uniquely suited for developing advanced Silicon–Carbon (Si–C) nanosystems, a material class of immense technological importance.

Si–C systems range from carbon-doped silicon and silicon carbide (SiC) to layered heterostructures like graphene-on-silicon. These materials exhibit exceptional properties: silicon provides a mature semiconductor platform, carbon (in its sp^2 -hybridized graphene form) offers high carrier mobility and thermal conductivity, and SiC presents remarkable hardness and wide-bandgap semiconducting behavior [4,5]. However, integrating these dissimilar materials with high interfacial quality and minimal defects poses a significant fabrication challenge. Conventional high-temperature chemical vapor deposition (CVD) for graphene, for instance, is often incompatible with pre-processed silicon devices [6].

This review examines LPD as a strategic solution to these challenges. We focus on its application in developing Si–C thin films, using graphene-silicon hybrids as a primary case study. Furthermore, we introduce two conceptual frameworks—**Self-Control Closed-Loop (SCCL) dynamics** and **Dynamic Fractal Space (DFS)**—to provide a deeper theoretical understanding of the non-linear, feedback-rich processes that define LPD. By linking process parameters to emergent material properties through these models, we aim to establish LPD as a rational design tool for next-generation thin-film devices in energy conversion, electronics, and beyond.

2. Fundamentals of Laser-Plasma Deposition for Si–C Systems

2.1. Process Mechanism and Key Parameters

The LPD process for Si–C films typically involves ablating a composite target (e.g., graphite, silicon-carbide, or alternating silicon and graphite) with a high-power laser (Fig. 1). The resulting plasma plume contains a mixture of atoms, ions, electrons, and small clusters of Si and C. The film's final composition and structure are determined during the subsequent condensation on the substrate, influenced by:

- **Laser Parameters:** Wavelength (UV lasers often provide better ablation efficiency), pulse duration (fs, ps, ns, or CW), fluence, and repetition rate.
- **Plasma Conditions:** Background gas (argon, nitrogen) and pressure, which can thermalize the plume and influence cluster formation.
- **Substrate Conditions:** Temperature, crystallographic orientation, and surface preparation.

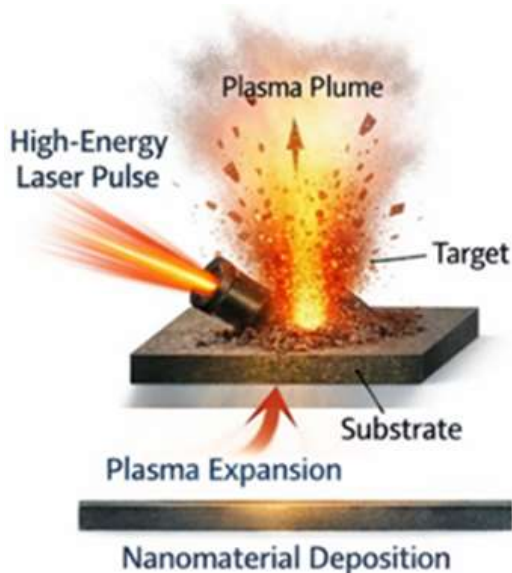


Figure 1. Laser–Plasma Deposition and Restructuring. Unified schematic combining: laser irradiation; plasma formation; transport; film formation on substrate.

2.2. Comparison with Other Thin-Film Techniques for Si–C

- **Chemical Vapor Deposition (CVD):** Excellent for large-area, high-quality graphene or SiC, but requires high temperatures ($>1000^{\circ}\text{C}$) and often involves hazardous precursors. Transfer steps for 2D materials can introduce contamination.

- **Sputtering:** Good for uniform, amorphous Si-C films (e.g., a-SiC:H for passivation), but limited in producing highly crystalline, phase-pure materials like graphene due to energetic particle damage.
- **LPD Advantages:** Offers *direct writing* capability, *low-temperature* crystalline growth (especially for graphene on silicon via CWLD [7]), excellent *stoichiometric control*, and the ability to create *graded or multilayer* structures in situ by target switching.

3. A Theoretical Framework for LPD: SCCL Dynamics and Dynamic Fractal Space

3.1. Self-Control Closed-Loop (SCCL) Dynamics in Film Growth

Traditional thin-film models treat deposition as a linear sequence of events. The SCCL framework conceptualizes it as a dynamic feedback system [8,9] (Fig. 2). During LPD, the *external operator* (laser energy) perturbs the system, but the growing film (the *operated system*) responds through processes like surface diffusion, island nucleation, and stress relaxation. This structural response alters the local chemical potential, work function, and adsorption sites, thereby *feeding back* into the ongoing condensation process of incoming plasma species. Stability is achieved through a dynamic balance, not a static endpoint. This explains the sensitivity of Si-C film properties (e.g., sp^2/sp^3 carbon ratio) to subtle changes in LPD parameters and substrate conditions.



Figure 2. Self-Control Closed-Loop (SCCL) Model. Block diagram: Energy input; Matter response; Feedback loop; Dynamic balance

3.2. Modeling Structural Evolution with Dynamic Fractal Space (DFS)

To describe the *spatial* evolution of the growing Si-C film within the SCCL framework, we employ Dynamic Fractal Space (DFS) [10,11]. In DFS, the material is represented as "knots" (atomic clusters) distributed within a fractal lattice (Fig. 3). The arrangement of these knots evolves over time under the

driving force of energy minimization dictated by the LPD conditions. The **effective fractal dimension (Df)** of the film becomes a state variable: a highly ordered 2D graphene sheet corresponds to $Df \rightarrow 2$, a porous nanocomposite film may have a non-integer Df between 2 and 3, and a dense amorphous SiC coating may exhibit a different topological signature. DFS provides a mathematical language to link LPD's energy input (laser fluence, wavelength) to the topological state of the resulting film.

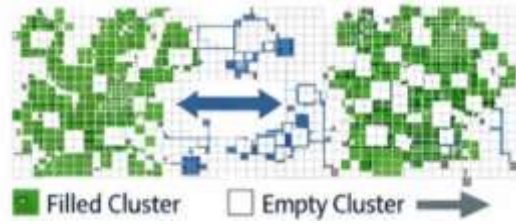


Figure 3. Dynamic Fractal Space (DFS) Representation. Fractal lattice with: empty clusters; knot migration; time arrow; visual hierarchy.

4. Case Studies in Si-C Thin-Film Development via LPD

4.1. Synthesis of Crystalline Graphene on Silicon Substrates

One of the most compelling demonstrations of LPD's restructuring power is the direct synthesis of graphene on silicon. Using a CWLD approach with a graphite target, a carbon-rich plasma is generated. Under optimized SCCL conditions (appropriate substrate temperature and laser power), the arriving carbon species self-organize into sp^2 -bonded hexagonal networks on the Si surface, bypassing the high-temperature requirement of CVD [12]. DFS models this as a plasma-to-solid transition where the system's effective fractal dimension converges toward that of a 2D sheet. Structural characterization via Raman spectroscopy and XRD confirms high-quality, few-layer graphene formation (Fig. 4).

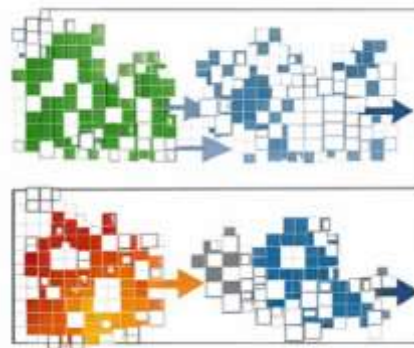


Figure 4. Graphene Clusters Formation

4.2. Growth of Silicon Carbide (SiC) and Nanocomposite Films

By ablating a stoichiometric SiC target or using alternating Si and C targets, LPD can produce SiC thin films. The phase (crystalline β -SiC vs. amorphous a-SiC) is controlled by the substrate temperature and laser parameters within the SCCL feedback loop. Furthermore, by tuning the plasma composition and background gas, nanocomposite films consisting of graphene nanocrystals embedded in an amorphous SiC matrix can be engineered. These composites are promising for hard coatings with tailored electrical conductivity [13].

5. Applications Enabled by LPD-Fabricated Si-C Thin Films

5.1. High-Efficiency Hybrid Photovoltaics

The integration of LPD-grown graphene as an active, rear-side layer in silicon solar cells creates a high-quality heterojunction. This graphene layer enhances carrier extraction, suppresses surface recombination, and improves thermal dissipation (acting as a heat-spreading layer) [14,15]. The SCCL-guided LPD process ensures an intimate, low-defect interface critical for these performance benefits, leading to enhanced open-circuit voltage and fill factor (Fig. 5,6).

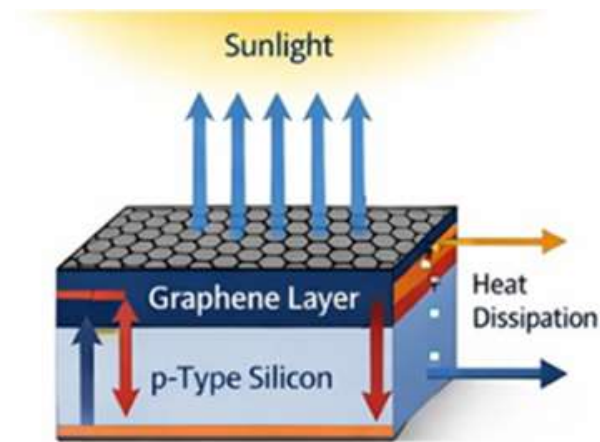


Figure 5. Graphene–Silicon Hybrid Device Concept. Caption emphasizes graphene as an active carrier-management layer. Schematic of: p-type Si absorber; rear graphene layer; carrier flow arrows; thermal dissipation paths.

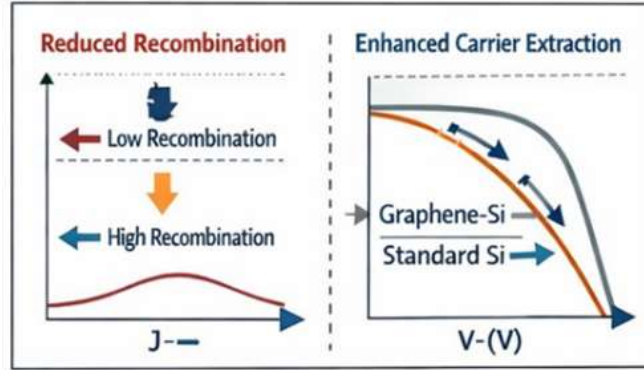


Figure 5. Impact on Photovoltaic Performance. Conceptual schematic plot (recombination suppression, carrier extraction enhancement, thermal stabilization)

5.2. Nanoelectronic and Spintronic Interfaces

The clean, abrupt interface achievable with LPD is vital for nanoelectronics. Graphene-on-silicon Schottky junctions with tunable barrier heights can be realized. For spintronics, the combination of silicon's long spin lifetime and graphene's high spin diffusion length creates a promising platform [16]. Precise control over the interfacial structure via LPD is essential for efficient spin injection and detection in such hybrid systems.

5.3. Functional Coatings and Sensors

Amorphous Si-C (a-SiC) films grown by LPD serve as excellent passivation and hard coating layers due to their chemical inertness, high hardness, and tunable optical bandgap. Nanocomposite Si-C films with embedded graphitic phases can be engineered for specific tribological or sensing applications, where the electrical conductivity changes in response to environmental stimuli.

6. Conclusions

Laser-plasma deposition has proven to be a uniquely powerful tool for the development of advanced Si-C thin films. Its integrated destructuring-restructuring mechanism, operating under non-equilibrium conditions, allows for the precise engineering of material phases, interfaces, and nanostructures that are difficult to achieve with conventional methods. The theoretical frameworks of SCCL dynamics and DFS provide a profound conceptual lens through which to understand, model, and

ultimately predict the outcomes of the LPD process, transforming it from an empirical art into a science-based design tool.

Future research directions should focus on:

1. **Scalability:** Advancing LPD systems for large-area, uniform deposition without compromising the unique structural benefits.
2. **In-Situ Diagnostics & AI Control:** Integrating real-time plasma and surface diagnostics with machine-learning algorithms to actively control the SCCL feedback loop, enabling the growth of films with pre-programmed properties.
3. **Expanded Material Space:** Applying the LPD-SCCL-DFS approach to other complex material systems, such as 2D transition metal dichalcogenides on semiconductors or multicomponent oxide-carbon composites.
4. **Novel Device Architectures:** Exploiting the design freedom offered by LPD to create three-dimensionally structured, multifunctional thin-film devices for energy storage, quantum computing, and bio-integrated electronics.

By embracing its dynamic and restructuring nature, laser-plasma deposition is poised to remain at the forefront of thin-film technology, enabling the next generation of high-performance nanosystems.

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LIBS Technology for Plasma Characterization:

Data Processing and Theoretical Analysis

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Abstract

Laser-induced breakdown spectroscopy (LIBS) enables rapid elemental and plasma diagnostics, yet its quantitative interpretation is constrained by the transient, non-uniform, and non-equilibrium nature of laser-induced plasmas. We present a combined experimental and theoretical study of LIBS plasmas generated on metallic targets, aimed at establishing a consistent diagnostic framework integrating spectroscopic measurements with deterministic–stochastic plasma modeling. Single-shot LIBS experiments were performed on six metals (Al, Cu, brass, Pb, stainless steel, and Ti) using a nanosecond Nd:YAG laser. Electron density and temperature were evaluated using Stark broadening, Boltzmann plots, and ionized-to-neutral line intensity ratios as an LTE-based Saha reference. To account for shot-to-shot variability and non-LTE effects, ionization–recombination kinetics were modeled using a stochastic extension of classical rate equations. The inclusion of stochastic fluctuations improves agreement with experimental spectra and enhances the robustness of plasma diagnostics. The results demonstrate the necessity of stochastic modeling for reliable LIBS analysis and highlight LIBS plasmas as compact testbeds for studying non-equilibrium plasma dynamics.

Introduction

Laser–matter interaction leading to plasma formation is a fundamental process underpinning a wide range of modern scientific and technological applications, from materials processing and surface engineering to plasma diagnostics and high-energy density physics. Among laser-based diagnostic techniques, laser-induced breakdown spectroscopy (LIBS) has emerged as a versatile and rapid tool for elemental analysis and characterization of transient plasmas generated by nanosecond laser pulses [1–3]. The method relies on optical emission from excited atoms and ions within the laser-induced plasma plume, providing simultaneous information about elemental composition and plasma parameters.

Despite its broad applicability, quantitative interpretation of LIBS spectra remains challenging. Laser-induced plasmas are inherently transient, strongly non-uniform in space and time, and often far from local thermodynamic equilibrium (LTE), especially during the early stages of plasma evolution [2–4]. Steep gradients of electron temperature and density, rapid expansion, and fluctuating electric microfields lead to spectral line broadening, self-absorption, and shot-to-shot intensity variations, which complicate reliable plasma diagnostics [5].

Classical LIBS analysis typically employs a combination of Stark broadening for electron density determination and Boltzmann plots for excitation temperature estimation, assuming optically thin emission and quasi-LTE conditions [1,4,6]. The Saha equation is frequently used as a baseline model for ionization balance, enabling indirect estimation of electron temperature from ionized-to-neutral line intensity ratios [6,7]. However, numerous studies have demonstrated that these equilibrium-based approaches can only provide approximate trends when applied to short-lived laser plasmas, where collisional–radiative processes and radiative losses violate LTE assumptions [8–10].

Recent advances in plasma spectroscopy emphasize the importance of treating laser-induced plasmas as non-equilibrium systems, in which deterministic transport processes coexist with stochastic fluctuations originating from microscopic ion–electron collisions and local field variations [11–13]. Such fluctuations manifest experimentally as shot-to-shot variability of emission intensities and line shapes, even under nominally identical experimental conditions. Purely deterministic kinetic models are therefore insufficient to reproduce the observed behavior of LIBS plasmas.

From a broader physical perspective, the dynamics of laser-induced plasmas share important similarities with processes encountered in high-energy-density and laser–plasma physics. Two-fluid descriptions, Langmuir oscillations, and fluctuation-driven instabilities play a central role both in microscale LIBS plasmas and in large-scale systems such as laser-driven plasma accelerators and fusion-

relevant plasmas [14–17]. Consequently, LIBS plasmas can be regarded as compact laboratory analogues for studying fundamental non-equilibrium plasma processes under well-controlled conditions.

In this context, the integration of deterministic plasma modeling with stochastic extensions provides a promising route toward improved LIBS diagnostics. Stochastic differential equation frameworks, solved numerically using methods such as Euler–Maruyama schemes, have proven effective in capturing fluctuation-driven dynamics in plasma and optical systems [18]. Applying such approaches to LIBS enables a more realistic description of ionization–recombination kinetics and improves consistency between modeled and experimental spectra.

The present work builds upon these developments by combining systematic LIBS experiments on metallic targets with a deterministic–stochastic modeling framework. By integrating Stark broadening, Boltzmann plots, and LTE-based Saha analysis with stochastic kinetic modeling, we aim to establish a coherent and physically grounded diagnostic methodology. Beyond applied spectroscopy, this approach contributes to the broader understanding of fluctuation-dominated, non-equilibrium plasmas relevant to high-energy physics and laser–plasma interaction

Problem Statement and Methodology

The specific objectives of this work are to: acquire reproducible LIBS spectra from a selected set of metallic targets under well-controlled experimental conditions and extract key plasma parameters from spectral line shapes and intensities.

Experiments were performed on six metallic targets: copper (Cu), brass (Cu–Zn), lead (Pb), aluminium (Al), stainless steel (Fe–Cr–Ni), and titanium (Ti). Sheets were pre-sorted by code, material, and thickness (0.1–0.5 mm) and their surfaces were cleaned immediately before ablation to reduce oxide/contamination effects (fig.1 b).

A Q-switched Nd:YAG laser ($\lambda = 1064$ nm, $\tau \approx 7$ ns, 1 Hz) was focused normal to the target with a 100 mm plano-convex lens. The ~ 100 μm spot size was verified by (CCD beam profiler), yielding a fluence of ~ 89 J cm $^{-2}$ at 70 mJ. Emission was collected at 45° with a $\varnothing$ 600 μm fiber and analyzed by a StellarNet BlackComet-SR spectrometer (200–1100 nm, ~ 1.5 nm) (fig.1. a)

The samples were placed and firmly mounted on a black ceramic substrate, which ensured stability and had a neutral influence on the spectrum (Fig.1. c). Thin samples (0.1 mm copper and brass) were additionally placed on a sacrificial substrate to prevent the risk of perforation or deformation by the laser.

All samples were observed under the same optical configuration to ensure the reliability of the comparative analysis.

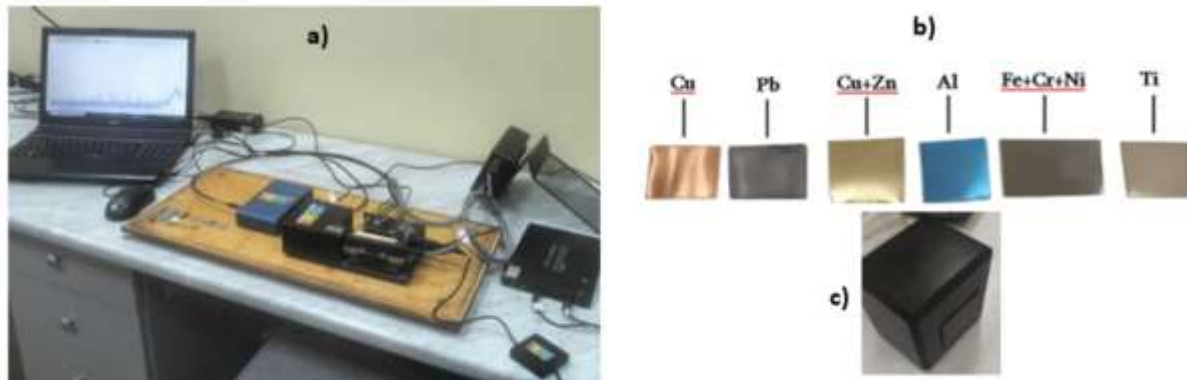


Figure.1. a) LIBS systems with blue wave (190-450 nm) spectrometer and YAG laser ($\lambda = 1064$ nm, $\tau \approx 7$ ns, 1 Hz), b) Approximately equal-size samples selected for analysis, c) Ceramic mounting block

The laser energy and other parameters were fixed, which significantly increased the importance of surface preparation and sample mounting. Several laser pulses were applied to each sample, and the resulting spectra were recorded in different wavelength ranges (189–410 nm). For each material, characteristic neutral and ionized lines were selected, as presented in Table 1.

Table 1. Main physical properties and characteristic LIBS spectral lines of analyzed metallic samples

№	Sample Name	Material (Chemical Formula)	Thickness (mm)	Density (g/cm ³)	Melting Point (°C)	Optical skin depth δ at 1064 nm (nm)	Main LIBS Spectral Lines (nm)	Key Properties
1	Copper	Cu	0.1	8.96	1085	8	324.7, 327.4, 510.5	High thermal and electrical conductivity; oxidizes quickly (clean before LIBS).
2	Lead	Pb	0.3	11.34	327	20-25	367.1, 373.9, 405.8	Very heavy and soft; easily pierced by the laser if thin; secure mounting required.
3	Brass (Copper + Zinc)	Cu + Zn (30–45% Zn)	0.1	8.4–8.7	900–940	12-18	Cu lines + Zn lines 213.9, 334.5, 468.0	Alloy of copper and zinc; golden-yellow color; good corrosion resistance.
4	Aluminium	Al	0.5	2.70	660	13	394.4, 396.1, 358.7	Lightweight; forms a stable oxide layer (affects spectrum, requires cleaning).
5	Stainless Steel	Fe + Cr + Ni (alloy)	0.3	7.7–8.0	1400–1450	20-30	Fe lines 248.3, 302.1, Cr/Ni lines	Strong, corrosion-resistant; magnetic response.
6	Titanium (Grade 2)	Ti	0.5	4.51	1668	18-22	334.9, 368.5, 399.	Light and strong; relatively weak LIBS intensity; must be tightly fixed.

The investigated targets (Al, Cu, brass, Pb, stainless steel, and Ti) exhibit markedly different thermal and electrical properties, which play a crucial role in laser–matter interaction and subsequent plasma formation. Their melting points, for example, span a wide range from 327 °C for lead to 1668 °C for titanium, implying substantial differences in ablation thresholds, heat diffusion, and crater morphology under identical laser irradiation conditions.

Beyond bulk thermal properties, the optical skin depth δ at the laser wavelength (1064 nm) is a key parameter governing the effective absorption and interaction zone at the target surface. For metals, the skin depth depends on the electrical conductivity σ and magnetic permeability μ according to

$$\delta = \sqrt{\frac{2}{\mu_0 \omega \sigma}},$$

where μ_0 is the vacuum permeability and ω the angular frequency of the incident radiation. For good conductors at 1064 nm, δ is typically on the order of several tens of nanometers. Consequently, the skin depth defines the initial energy-deposition volume and, together with thermal transport processes, strongly influences crater formation and the early-time thermodynamic state of the laser-induced plasma.

Spectra were acquired in single-shot, time-integrated mode. For each target material, three independent laser shots were recorded under identical experimental conditions. The samples were rigidly clamped on a black ceramic mount to ensure a constant focal plane and reproducible laser–target geometry. Thin foils (0.1 mm Cu and brass) were placed on a sacrificial ceramic backing to prevent perforation and to enhance lateral heat spreading. Since a rotating or translating target holder was not employed, the impact point was shifted laterally by at least 0.2–0.5 mm between successive shots in order to avoid crater overlap and local overexposure.

For each recorded spectrum, characteristic emission lines were identified. Peak wavelengths were determined with a precision of ± 0.1 nm based on prior wavelength calibration, and line intensities (arbitrary units) were taken as peak heights after local baseline subtraction. To enable meaningful comparison between different materials, intensities were normalized to the mean value of the three replicates for each target, thereby reducing variability arising from minor differences in surface condition and sample thickness. The extraction of full widths at half maximum (FWHM) and correction for instrumental broadening are addressed separately in the Stark broadening analysis section.

For copper, three single-shot spectra acquired under identical conditions (Fig. 2) demonstrate high reproducibility. The dominant Cu I lines at 324.7 nm and 327.4 nm are consistently observed, with residual shot-to-shot intensity scatter below 5%, attributable primarily to surface roughness and small

variations in the ablation spot position. Brass (Cu–Zn) spectra are similarly reproducible and exhibit the expected Cu I lines at 324.7 nm and 327.4 nm, together with prominent Zn I lines at 213.9, 334.5, and 468.0 nm. In this case, the shot-to-shot intensity scatter remains below 7%, reflecting minor differences in ablation location and surface microstructure.

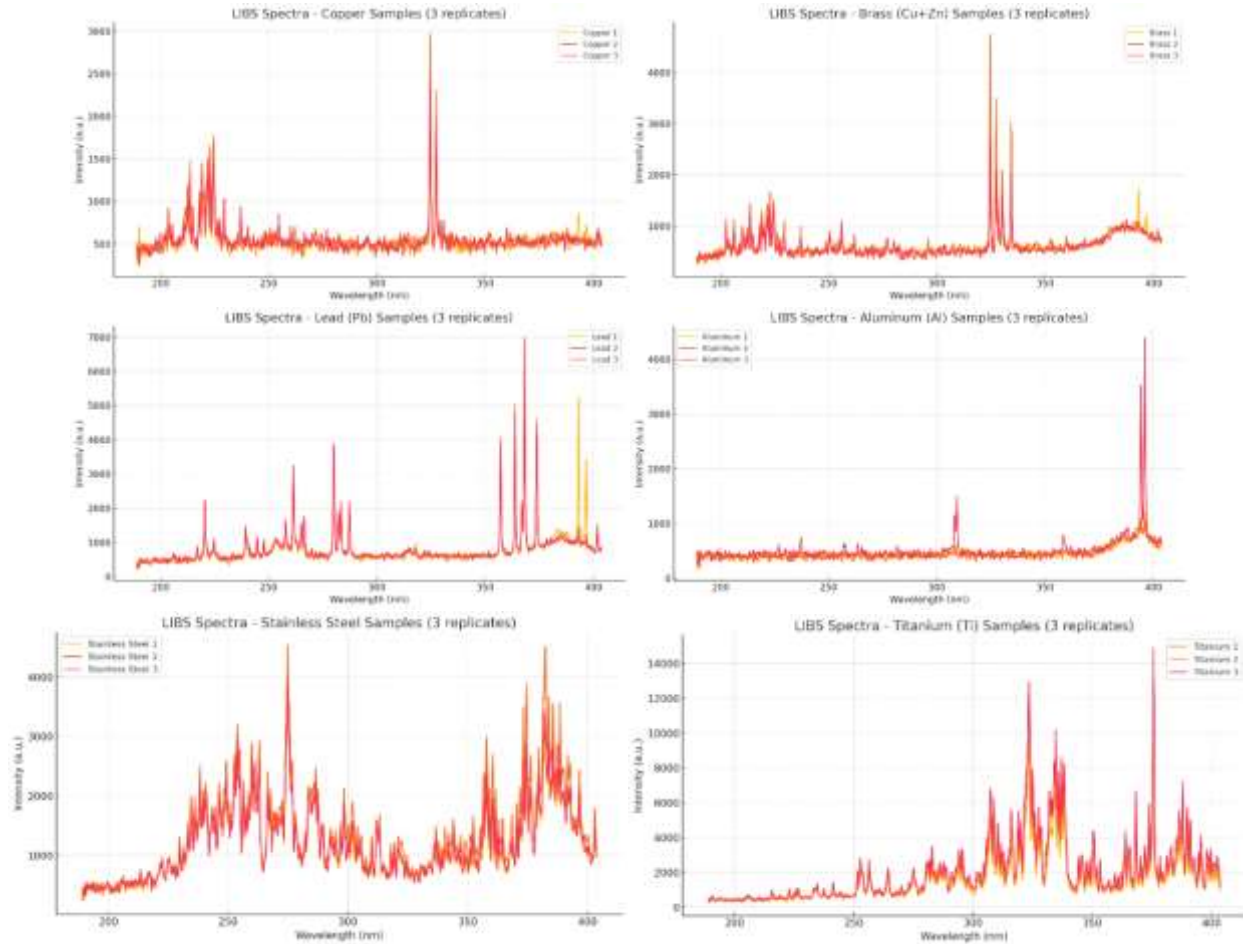


Figure 2. Spectral profiles of three single-shot replicate measurements for each sample

For lead (Pb), the most intense spectral features correspond to neutral lead (Pb I) lines near 367.1, 373.9, and 405.8 nm. The replicate spectra show excellent reproducibility, with intensity variations below 6%, mainly due to small variations in surface roughness and ablation-spot placement. Aluminium spectra are dominated by Al I lines at 394.4 nm and 396.1 nm, along with the Al II line near 358.7 nm. The reproducibility is similarly good, with shot-to-shot intensity scatter below 8%, which can be attributed to variations in ablation microstructure and the presence of a native oxide layer.

Stainless steel (Fe–Cr–Ni) spectra exhibit characteristic Fe I lines at 248.3 nm and 302.1 nm, Cr I at 357.9 nm, and Ni I at 341.5 nm. The recorded spectra are highly reproducible, with intensity scatter below 7%. Titanium spectra are dominated by Ti I lines near 334.9, 368.5, and 399.9 nm. In this case, reproducibility remains high, with shot-to-shot intensity variations below 9%, primarily associated with native oxide layers and small differences in ablation-spot morphology.

Neutral (I) and ionized (II) emission lines were identified by cross-referencing the measured peak centroids with standard atomic data. The NIST Atomic Spectra Database (ASD) was used as the primary reference source, complemented by spectral atlases and the handbook of Cremers and Radziemski. Initial line matching was performed using air wavelengths with a tolerance of ± 0.2 – 0.3 nm. Subsequently, assignments were validated by checking the corresponding upper and lower energy levels, transition probabilities ($A_{ki} / \log gf$), and the presence of companion lines belonging to the same multiplet.

Given the instrumental full width at half maximum (FWHM) of approximately 1.5 nm and the wavelength calibration accuracy, the uncertainty in peak-centroid determination was limited to $\leq \pm 0.1$ nm, which justifies the adopted matching tolerance. Line intensities were obtained as peak heights after local baseline subtraction.

The following procedural rules were applied to ensure reliable line selection:

- Emission lines known to be strongly self-absorbed or severely blended were excluded from further analysis, or deconvolved when justified by sufficient signal-to-noise ratio.
- For wavelengths below 200 nm, appropriate vacuum-to-air wavelength conversions were applied. Within the present spectral range (200–1100 nm), all wavelengths are reported as air wavelengths, consistent with the NIST ASD.

Representative examples of assigned lines include Cu I at 324.7 and 327.4 nm with Cu II near 213.6 nm, and Al I at 394.4 and 396.1 nm with Al II near 358.7 nm. This identification workflow yielded a robust and reproducible line list, enabling subsequent analysis based on ion-to-neutral intensity ratios ($I_{\text{ion}}/I_{\text{neutral}}$), Stark-broadening-derived line widths, and an LTE-based Saha reference for plasma parameter inference, with non-LTE limitations explicitly acknowledged.

Using the LTE Saha relation in conjunction with the measured ion-to-neutral intensity ratio $I_{\text{ion}}/I_{\text{neutral}}$, the average values reported in Table 2 serve as a baseline proxy for the ionization balance n_{i+1}/n_i at the measured electron density n_e . Higher ratios (e.g., Al, Cu, and brass) correspond to larger ionization fractions n_{i+1}/n_i and, under otherwise similar conditions, to higher electron

temperatures T_e . Conversely, lower ratios observed for Pb, Ti, and stainless steel indicate smaller ionization fractions and lower T_e .

Table 2. Identification of neutral (I) and ionized (II) emission lines and average ionization ratios ($I_{\text{ion}}/I_{\text{neutral}}$) for the analyzed materials

Material (Sample)	Neutral line (nm)	Ionized line (nm)	Average ratio $I_{\text{ion}}/I_{\text{neutral}}$
Copper (Cu)	324.7 (Cu I)	213.6 (Cu II)	0.35–0.40
Brass (Cu–Zn)	324.7 (Cu I)	213.6 (Cu II) (+ Zn II 334.5)	0.38–0.42
Lead (Pb)	367.1 (Pb I)	220.4 (Pb II)	0.30–0.35
Aluminium (Al)	394.4, 396.1 (Al I)	358.7 (Al II)	0.40–0.50
Stainless steel (Fe–Cr–Ni)	302.1 (Fe I)	259.9 (Fe II)	0.25–0.30
Titanium (Ti)	368.5 (Ti I)	337.3 (Ti II)	0.30–0.35

These material-dependent trends are consistent with electron densities derived independently from Stark broadening analysis and with the selection of diagnostic lines exhibiting minimal self-absorption. It is emphasized that this interpretation relies on the assumption of local thermodynamic equilibrium and is intended to capture relative trends rather than absolute plasma parameters. Accurate determination of ionization balance under non-LTE conditions would require a full collisional–radiative treatment.

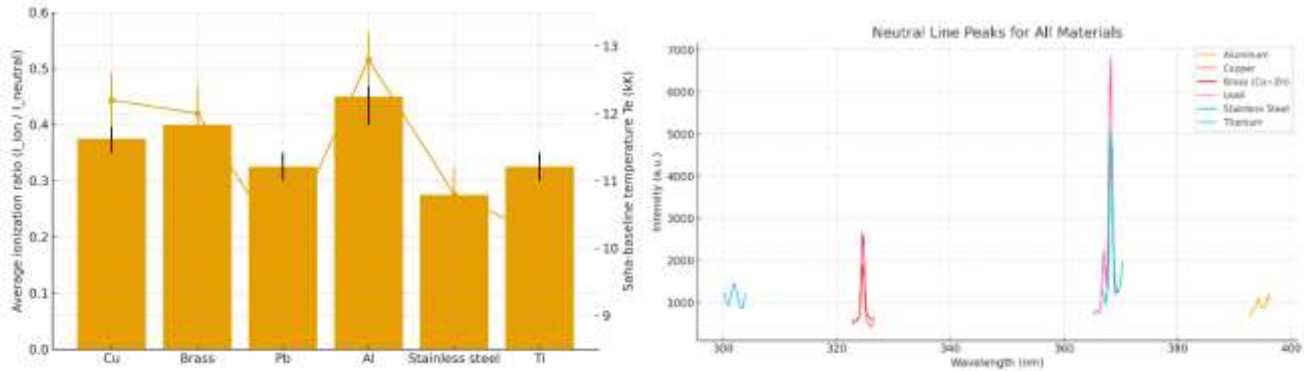


Figure 3. a) Average ionization ratios vs estimated electron temperature for each material, b) Neutral line peaks for all materials

Fig.3 a) compares, for each material, the average intensity ratio $I_{\text{ion}}/I_{\text{neutral}}$ (blue bars; Eq. 22) with the electron temperature T_e (red line) inferred from the LTE Saha relation using the measured n_e . Materials with higher $I_{\text{ion}}/I_{\text{neutral}}$ (e.g., Al, Cu, brass) show larger ionization fractions n_{i+1}/n_i and T_e values of about 12–13 kK; stainless steel and Pb/Ti exhibit comparatively lower ratios and $T_e < 11$ kK,

consistent with a lower degree of ionization. These trends are intended as an LTE baseline; absolute non-LTE values would require a collisional–radiative treatment.

Electron density was obtained from Stark broadening of selected, optically thin neutral lines (e.g., Cu I 324.7 nm, Al I 394.4 nm, Pb I 367.1 nm). For lines with a linear Stark parameters ω are quoted in nm per 10^{16} cm^{-3} :

$$\Delta\lambda_{1/2}^{Stark} \approx 2\omega \left(\frac{n_e}{10^{16} \text{ cm}^{-3}} \right) \rightarrow n_e = \frac{\Delta\lambda_{1/2}^{Stark}}{2\omega} \cdot 10^{16} \text{ cm}^{-3}$$

where ω is the tabulated Stark width parameter for the specific transition. When available, the weak T_e -dependence of ω was applied within the 10^{-13} kK range. This procedure yields n_e values used in Fig.3 a) to compute the corresponding T_e from the Saha baseline.

Fig.3 b) overlays the principal neutral lines for all six materials under identical conditions to highlight differences in line width (FWHM) and relative intensity. The selected transitions are Cu I 324.7 nm, Al I 394.4 nm, Pb I 367.1 nm, Fe I 302.1 nm (stainless steel), Ti I 368.5 nm, and Cu I 324.7 nm for brass (Cu–Zn). For visual comparability, profiles are shown on the same wavelength scale and normalized to unit peak height; thus, broader traces directly indicate larger Stark widths (and hence higher n_e), while narrower traces correspond to lower n_e .

The Boltzmann method estimates the electron temperature from relative line intensities of a single element and charge state under (quasi-)LTE and optically thin conditions (minimal self-absorption and blending). The population of the upper level N_u follows:

$$N_u = \frac{N g_u}{Z(T)} e^{-E_u/(k_B T)}$$

where N is the total population of the species, g_u the level degeneracy, E_u the upper-level energy, $Z(T)$ the partition function, and T the (excitation) temperature. For an optically thin line $u \rightarrow l$:

$$I_{ul} \propto N_u A_{ul} h\nu,$$

so that:

$$\ln \left(\frac{I_u \lambda}{g_u A_{ul}} \right) = -\frac{E_u}{k_B T} + \text{const.}$$

Thus, plotting $y = \ln \left(\frac{I_u \lambda}{g_u A_{ul}} \right)$ versus $x = E_u$ yields a straight line with $\text{slope} = -\frac{1}{k_B T}$. The temperature inferred from the slope is reported as T_e (Fig. 3 b).

For Boltzmann plots we selected 3–6 unblended lines of the same element and ionization stage (λ , E_u , A_{ul} , g_u from NIST). After baseline subtraction we used integrated line areas (or peak heights when

SNR was limited) and excluded lines showing self-absorption or blends. Electron temperature T_e was obtained from the slope of $\ln(I\lambda/(gA))$ vs E_u ; only fits with good linearity (e.g., $R^2 \geq 0.95$) were accepted.

As a result, T_e for materials with few usable neutral lines carries a larger uncertainty; this underscores the need for well-defined, sufficiently intense lines when applying the Boltzmann-plot method (see Table 3).

Table 3: Estimated Electron Temperatures (T_e) Using the Boltzmann Plot Method

Material	T_e (kK)	Reliability
Aluminium (Al)	~28.1	High (strong lines)
Copper (Cu)	~4.9	Low (limited lines)
Brass (Cu+Zn)	~16.4	Medium
Lead (Pb)	~1.4	Low (weak lines)
Stainless Steel	<i>Unreliable</i>	Very low (weak/overlapping lines)
Titanium (Ti)	~2.4	Low (weak lines)

Conclusion

In this work, we developed and experimentally validated a deterministic–stochastic framework for modeling ionization–recombination dynamics in laser-induced plasmas and directly linked it to standard LIBS diagnostics. Because single-shot, time-integrated LIBS spectra originate from plasmas that are strongly non-uniform in space and time, a consistent interpretation requires the combined use of complementary diagnostics. By integrating Stark broadening for electron density determination, an LTE-based Saha relation for ionization trends at the measured n_e , and Boltzmann plots for excitation temperature T_{exc} , a coherent and physically consistent picture of the plasma state was obtained.

The results demonstrate that stochastic fluctuations in ionization–recombination processes play a decisive role in the accuracy and reliability of plasma diagnostics. Materials with higher ionization propensity, such as aluminium, copper, and brass, exhibit Saha-based electron temperatures of approximately 12–13 kK, whereas lead, titanium, and stainless steel show lower values below 11 kK. Stark broadening analysis reveals the highest electron densities for aluminium and stainless steel, while brass and copper yield comparatively lower values; for lead, the limited line quality prevents reliable n_e extraction. Ionization ratios follow the same material-dependent trends, with the highest

values observed for aluminium and copper and the lowest for stainless steel. Excitation temperatures derived from Boltzmann plots are most reliable for aluminium and brass, whereas weak or overlapping lines limit their applicability for the remaining materials.

The Saha-based results presented here should be regarded as an LTE reference; accurate absolute values under non-LTE conditions will require full collisional–radiative modeling. Future work will focus on time-resolved gated detection, optimization of fluence and delay parameters, improved spectral resolution, and implementation of a collisional–radiative solver, with the goal of extending the present framework toward fully quantitative analysis of complex, multi-element materials.

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Synchrotron radiation photoemission study of the electronic structure of the ultrathin Na/GaN interface

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Abstract

The electronic surface structure of GaN samples grown by plasma-assisted molecular beam epitaxy was studied using synchrotron photoelectron spectroscopy in the photon energy range of 75–770 eV. Experiments were carried out directly under ultrahigh vacuum conditions with submonolayer sodium coverages on the gallium nitride surface. Analysis of the photoemission spectra in the valence band region and the spectra of the Ga 3*d* and N 1*s* core levels at various excitation energies revealed that sodium adsorption leads to a decrease in the spectral intensity and a shift toward higher binding energies, indicating a transformation of the near-surface energy band bending and a change in the surface potential. Sodium adsorption on GaN was found to induce the appearance of new surface states localized in the bandgap region of the sample. The observed spectral changes were found to be due to charge transfer between the adsorbed sodium layer and gallium or nitrogen atoms on the sample surface.

Introduction

Gallium nitride (GaN) is a wide-bandgap semiconductor with an exceptional set of electrical and optical properties. These include high mobility and critical breakdown field strength, thermal stability, and radiation resistance. Due to its direct-bandgap structure and the ability to vary the bandgap width

when creating solid solutions, GaN is of great interest for fundamental condensed matter physics and applied microelectronics. In particular, it is a key material for the creation of next generation high-frequency power electronics, as well as highly efficient light-emitting diodes and lasers covering a broad spectral range – from deep ultraviolet to infrared radiation [1].

Currently, the primary focus in the development of GaN technologies has shifted toward improving the reliability and ultimate performance of devices. A key barrier to this endeavor remains the production of structurally perfect epitaxial layers characterized by a minimal density of dislocations and stacking faults, which critically impact degradation processes and the quantum efficiency of devices [2]. Imperfections in the crystal structure of epitaxial layers lead to undesirable leakage currents and a reduced service life of semiconductor systems. Therefore, a detailed study of epitaxy mechanisms and the structural parameters of the layers is a priority.

Traditionally, sapphire, silicon, and silicon carbide are used as substrates for GaN growth. However, significant differences in their crystal lattice parameters and thermal expansion coefficients complicate the formation of defect-free films on these materials. To minimize the negative influence of the heterojunction and compensate for structural mismatch, specialized buffer layers are required. The use of homoepitaxial substrates (GaN) avoids these problems, but their widespread adoption is limited by their high cost. An optimal alternative is the use of GaN templates pre-grown by metal-organic chemical vapor deposition (MOCVD) on readily available commercial substrates. In modern gallium nitride-based electronics, the (0001) surface orientation dominates, necessitating a detailed analysis of its physicochemical properties. Creating a high-quality metal/semiconductor contact is an equally important task in device design. The characteristics of this interface determine the electrical parameters and overall operational reliability of microelectronic devices. The electronic structure of the film/GaN interface is influenced by both the initial state of the semiconductor surface and the properties of the adsorbed layer. Interaction with adsorbed atoms can significantly modify the surface characteristics of the system.

The problems of the electronic structure of the gallium nitride surface and the detailed mechanisms of adsorption of various chemical elements, especially alkali metals, have long been the focus of attention in the scientific community. The fundamental principles of these processes have been described in detail in many theoretical and experimental studies [3-6]. The review [7] deserves special mention, as it systematizes a vast amount of calculated data concerning the stability of various surface reconstructions and the binding energies of adsorbates. In addition, a number of studies [8-12] have thoroughly

investigated the photoemission characteristics and the evolution of energy bands during the formation of Cs/GaN, K/GaN and Li/GaN interfaces, which made it possible to identify general patterns of changes in the electronic structure upon contact with alkali metals. Despite the extensive study of related systems, the Na/GaN interface remains less studied, although a theoretical calculation performed within the framework of density functional theory (DFT) [13] indicates its high technological significance. In particular, it has been shown that sodium adsorption can radically modify the electronic properties of graphene-like gallium nitride (g-GaN), significantly increasing its sensitivity and selectivity to simple gas molecules. This opens the prospect of creating highly efficient next-generation gas sensors. However, until now, systematic experimental data on the behavior of the Na/GaN system under ultrahigh vacuum conditions have been almost non-existent. Preliminary studies of the Na/GaN interface were conducted in [14, 15]. Calculations in [15] showed that the adsorption of a thin coating (0.25 monolayer) of Na has an insignificant effect on the valence band spectrum, with the main changes observed near the Fermi level.

In this study, photoelectron spectroscopy (PES) using synchrotron radiation is used to study the electronic structure of the GaN surface and the evolution of the Na/GaN interface. PES was chosen as the primary research method due to its effectiveness in analyzing the band structure and determining the fundamental electronic characteristics of materials.

Experimental section

Gallium nitride samples were grown by nitrogen plasma-activated molecular beam epitaxy (PAMBE) on a Veeco GEN200 setup. Standard GaN/c-Al₂O₃ MOCVD templates with a thickness of ~2 μm were used for synthesis. Before the epitaxial process, the surface of the virtual substrate was degreased. Nitridization of the template was carried out directly in the growth chamber for an hour at a temperature of 870 K, after which the surface was cleaned by multiple deposition of gallium according to the established method [16]. The layers were synthesized at a substrate temperature of 960 K; the gallium flux was approximately 0.25 $\mu\text{m}/\text{h}$, and the nitrogen flux was 0.05 $\mu\text{m}/\text{h}$. According to the Hall effect data, the charge carrier concentration in the obtained samples at room temperature was close to $2 \times 10^{17} \text{ cm}^{-3}$. The thickness of GaN films grown by the PAMBE method on a GaN/c-Al₂O₃ template was ~200 nm, according to scanning electron microscopy data (see Fig. 1a). The surface quality of the grown GaN layers (see Fig. 1b), as well as the practically invisible interface between the GaN-PAMBE and GaN-MOCVD layers, are shown in Figs. 1a and 1b, confirming the correctness of the chosen growth resumption procedure on the template.

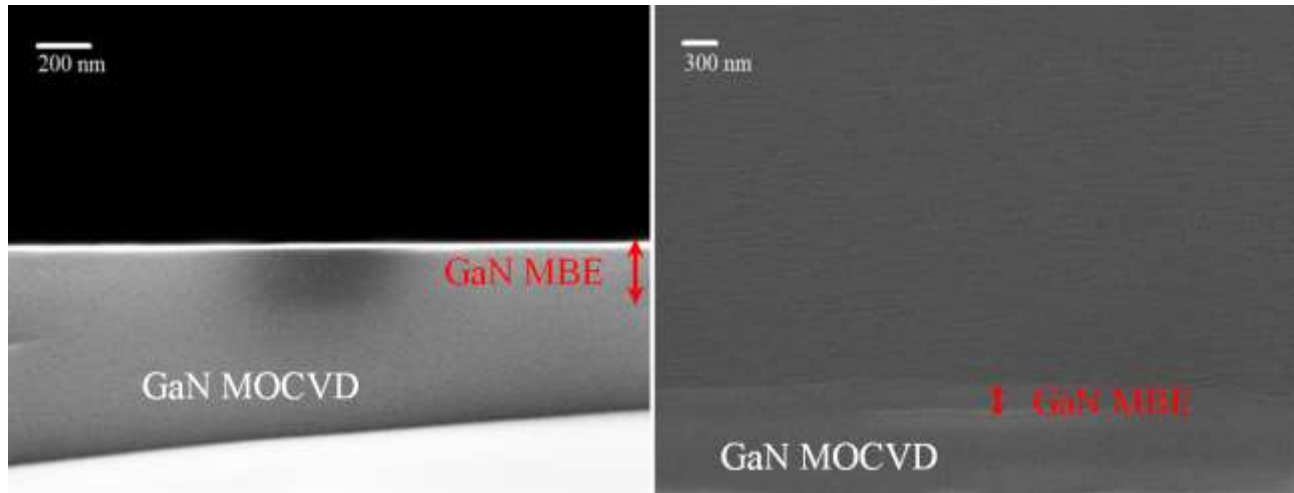


Figure 1. Scanning electron microscopy image of cross-sections of the GaN/template-GaN sample.

PES experiments were performed at the Russian-German synchrotron radiation beamline of the BESSY II storage ring (Berlin). Measurements were performed *in situ* under ultrahigh vacuum conditions of 5×10^{-10} Torr at room temperature in the photon energy range of 75–770 eV. The samples were pre-annealed at a temperature of approximately 870 K. The spectra showed only traces of oxygen (O 1s) and carbon (C 1s). The prepared surface was subsequently coated with atomically pure sodium using a standard evaporator. The energy scale of all presented spectra was calibrated relative to the Fermi level (E_F), and background correction was performed using the Shirley method.

Results and discussion

Figure 2 shows the photoemission spectra in the valence band region for a clean GaN surface at different excitation energies from 100 to 150 eV. The energy position of the valence band maximum on the surface (E_{VBM}) was determined by linear approximation of the leading edge of the valence band spectrum. The spectrum of the clean GaN surface is characterized by a structured photoemission band. The shape and width of the valence band spectrum are in good agreement with the results of photoemission studies published previously [9-12].

Using the Tanuma, Powell, and Penn (TTP-2M) equation [17], the photoelectron escape depth λ was calculated for two extreme cases. $\lambda = 5.38 \text{ \AA}$ and $5.95 \text{ \AA}$ for electrons with kinetic energy $E_{kin} = 100 \text{ eV}$ and 150 eV , respectively. It should be emphasized that for GaN, the λ value calculated using the TTP-2M equation is 30% higher than that determined from experimental data [18]. With increasing excitation

energy, the photoemission intensity increases in the binding energy range of ~ 5 eV and ~ 10 eV. It can be assumed that this occurs due to an increase in the probing depth. The position of the valence band edge on the surface E_{VBM} relative to the Fermi level (~ 3.0 eV) was also determined. The GaN sample has n -type conductivity, so the Fermi level is located near the conduction band in the bulk. Thus, upward band bending occurs on the sample surface, which is consistent with the results of [12].

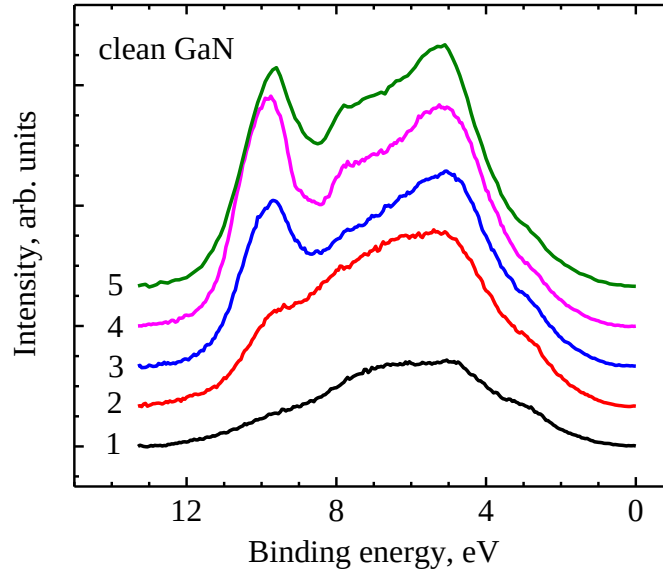


Figure 2. Photoemission spectra in the valence band region for a clean GaN surface at different excitation energies $h\nu$: 100 eV (1), 120 eV (2), 130 eV (3), 140 eV (4) and 150 eV (5).

Figure 3a shows the photoemission spectra in the valence band region for a GaN sample (1) and for the Na/GaN interface (2) with an Na coverage of 0.6 monolayers (ML) at an excitation energy of $h\nu = 130$ eV. Upon Na adsorption on the GaN surface, the intensity of the peaks of hybridized states in the valence band region decreases. Figure 3b shows the spectrum corresponding to the difference in photoemission intensities from a GaN surface coated with Na (Fig. 2a, curve 2) and from a clean GaN surface (Fig. 2a, curve 1). The difference spectrum allows us to visualize the main change in the electronic structure upon Na adsorption. Suppression of the two main maxima of the valence band is observed. The appearance of surface states at binding energies of 0–2 eV, induced by Na adsorption, was also detected. This result is in good agreement with the DFT calculation, which showed that the main changes in the electronic structure of GaN upon sodium adsorption occur in the Fermi level region [15].

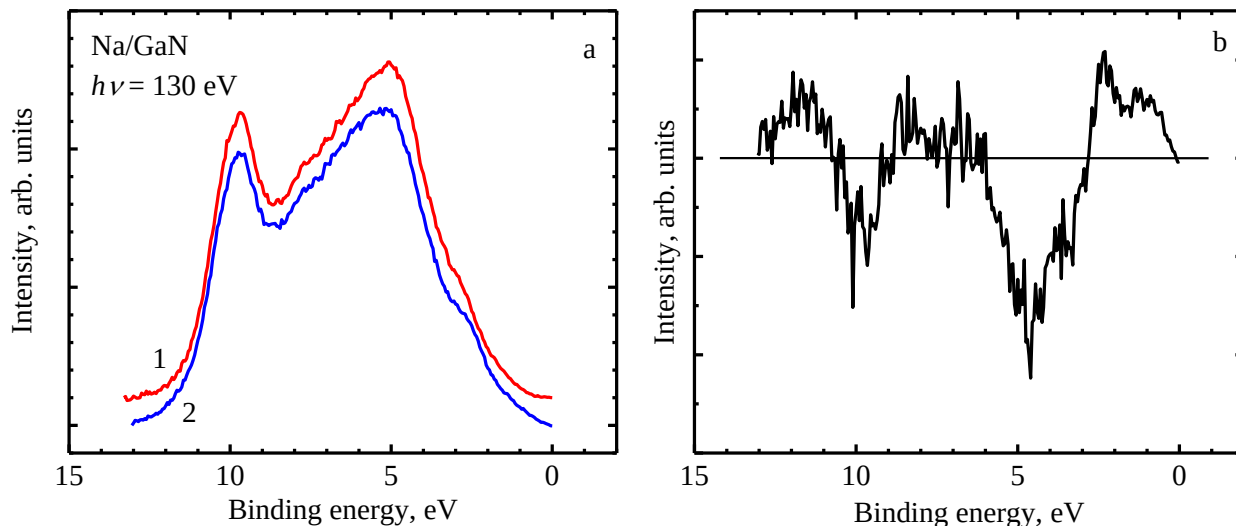


Figure 3. (a) Photoemission spectra in the valence band region for a clean GaN surface (1) and for the Na/GaN interface at 0.6 ML coverage (2). (b) Difference spectrum for the Na/GaN interface at 0.6 ML Na coverage and a clean GaN sample. Excitation energy $h\nu = 130$ eV.

Figure 4 shows the photoemission spectra of the Ga 3d core level for a clean GaN surface and Na/GaN interfaces obtained at excitation energies $h\nu$ equal to 150 eV (a) and 460 eV (b). The spectrum of the Ga 3d core level measured at a photon energy of 150 eV has a higher surface sensitivity compared to the data at 460 eV due to a smaller electron escape depth. The obtained results are almost completely consistent with the known literature data. The binding energy of the Ga 3d core level is 20.65 and 20.75 eV at excitation energies of 150 and 460 eV, respectively. A slight discrepancy in the binding energy values (0.1 eV) is due to the difference in excitation energies and, consequently, to variations in the sample probing depth. The feature (“shoulder”) in the region of high binding energies of Ga 3d is an intrinsic characteristic of the material and is associated with the bulk hybridization of the *d*- and *s*-states of the Ga-N bond [14]. A low-intensity peak corresponding to Ga-O bonds may also be present in this energy region. Sodium deposition leads to a decrease in the intensity of the Ga 3d core level peak by $\sim 14\%$ at an excitation energy of $h\nu = 150$ eV and by 3% at $h\nu = 460$ eV. This difference is explained by the different escape depths of the detected electrons for these energies. The peak shape remains unchanged. Sodium adsorption initiates a shift of the core levels toward higher binding energies, indicating a change in the surface band bending. The Ga 3d peak shift is 0.25 eV for excitation energies of 150 eV and 460 eV.

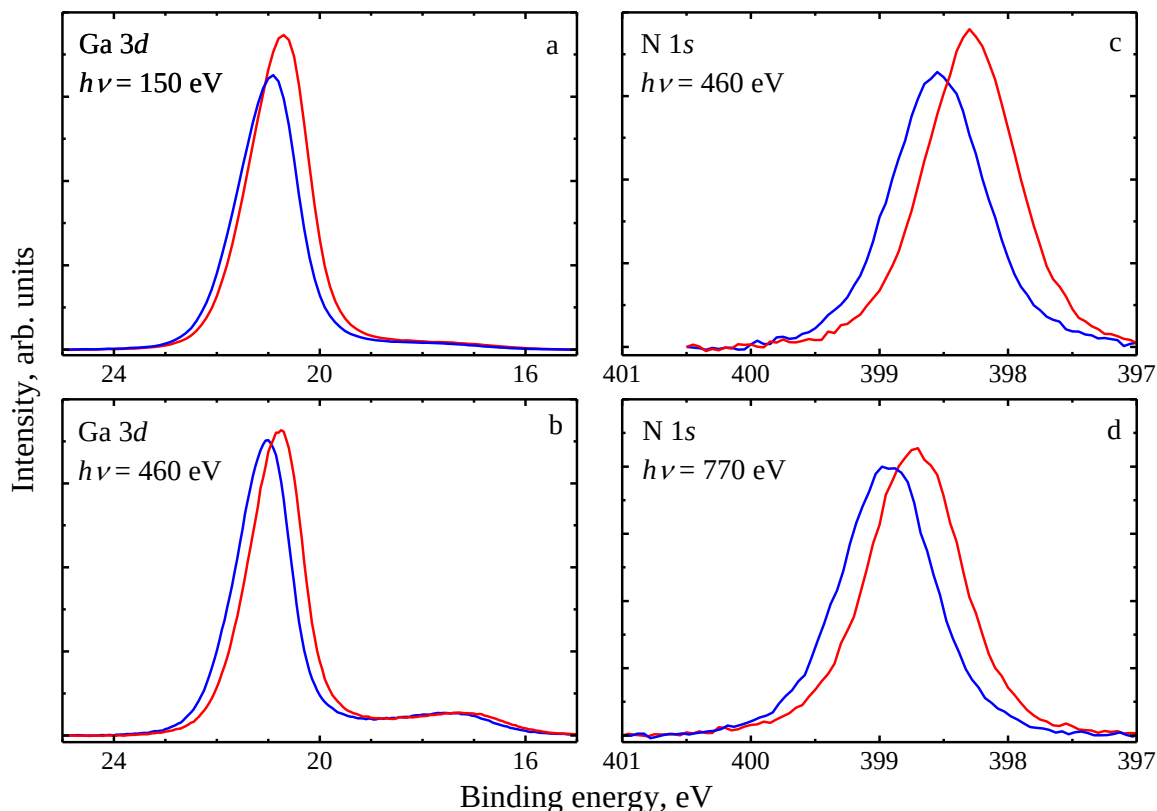


Figure 4. The photoemission spectra of the Ga 3d core level for a clean GaN surface and for the Na/GaN interface with Na coverage 0.6 ML at various excitation energies of 150 eV (a) and 460 eV (b). The photoemission spectra of the N 1s core level for a clean GaN surface and for the Na/GaN interface with Na coverage 0.6 ML at various excitation energies of 460 eV (c) and 770 eV (d). Red line – for clean GaN surface, blue line – for Na/GaN interface.

Figures 4c and 4d also show the N 1s core level photoemission spectra for a clean GaN surface and the Na/GaN interface at different excitation energies. The N 1s core level spectrum obtained at an excitation energy of 460 eV has a higher surface sensitivity compared to the spectrum at 770 eV, since a smaller depth is probed. The N 1s core level binding energy (398.7 eV), measured at an excitation energy of $h\nu = 770$ eV, is 0.4 eV higher, since photoemission occurs from greater depths of the sample. Sodium adsorption on the GaN sample surface is accompanied by a decrease in the N 1s peak intensity by 10% ($h\nu = 460$ eV) and 5% ($h\nu = 770$ eV) at a coverage of 0.6 ML.

Na adsorption initiates a shift of the core levels to higher binding energies, indicating a change in band bending. The maximum shift of the N 1s peak (0.25 eV at an energy of 460 eV) is achieved at a coverage of 0.6 ML. The observed shifts of the Ga 3d and N 1s levels are due to charge redistribution in the GaN surface bilayer as a result of the interaction of gallium and nitrogen atoms with adsorbed sodium

atoms. Analysis of the dynamics of the Ga 3*d* and N 1*s* peak intensities after adsorption indicates that the most favorable interaction is between sodium and nitrogen atoms in the GaN surface bilayer. Thus, the preferred adsorption sites for sodium atoms are the position above the surface N atoms and the hollow position [15].

Conclusion

GaN epitaxial layers were synthesized on GaN/c-Al₂O₃ substrates using plasma-assisted molecular beam epitaxy. Synchrotron radiation-based photoelectron spectroscopy was used for a comprehensive analysis of the electronic structure of the GaN surface and the evolution of the Na/GaN interface. Upward band bending was observed for the initial GaN surface. Upon reaching sodium coverage of 0.6 ML, a transformation of the near-surface energy band bending and a change in the surface potential occurred. The evolution of the core level spectra with increasing sodium coverage indicates high adsorption activity of the gallium nitride surface. Na atoms were found to be adsorbed predominantly on surface N atoms and in the hollow position. Sodium adsorption was found to initiate the formation of new surface states localized in the semiconductor's bandgap, indicating strong electronic hybridization. A medium decrease in the intensity of the core level peaks was observed, due to the adsorption process and possible screening of substrate photoelectrons by the adsorbed sodium layer. It was established that the observed spectral changes and electron density rearrangement are due to efficient charge transfer processes between electropositive Na atoms and surface gallium and nitrogen atoms. This interaction leads to a redistribution of electron density in the surface layer.

Acknowledgments

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Laser Based Vibrational Spectroscopy of Magnetically Enhanced ATP Hydrolysis: The Interplay of Ferromagnetic Nanosystems and Ion Catalysis

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Abstract

The external manipulation of adenosine triphosphate (ATP) hydrolysis, the central energy-releasing reaction in biology, presents a transformative strategy for modulating cellular bioenergetics. This study investigates the novel use of ferromagnetic nanoparticles (FNPs) and magnetic ions as activators of this fundamental process. We synthesized iron oxide (Fe_3O_4) and manganese ferrite (MnFe_2O_4) nanoparticles and systematically evaluated their effects on ATP hydrolysis through three distinct, yet potentially synergistic, mechanisms: (i) localized nanoscale heating via alternating magnetic field (AMF) exposure, (ii) mechanical actuation of the molecular environment, and (iii) the catalytic activity of released Fe^{2+} and Mn^{2+} ions. Vibrational spectroscopy (Raman and FTIR) served as a critical analytical tool to probe associated molecular-level changes. Our results demonstrate a 2.5-3 fold increase in non-enzymatic hydrolysis rates under AMF-induced hyperthermia, surpassing bulk heating effects. Isothermal AMF exposure in enzymatic assays revealed a ~40% activity enhancement, attributing to mechanical nanoparticle actuation. Furthermore, Mn^{2+} ions exhibited a pronounced catalytic effect. Spectroscopic data confirmed a weakening of ATP's γ -phosphate bond in the presence of magnetic species. This work establishes a foundational bridge between ferromagnetic nanomaterials and cellular biophysics, outlining a versatile platform for magnetically controlling energy pathways with significant implications for therapeutic strategies in oncology and bioenergetic research.

Keywords: Ferromagnetic nanoparticles; ATP hydrolysis; Magnetic hyperthermia; Nanoscale actuation; Vibrational spectroscopy; Manganese ions; Bioenergetics.

1. Introduction

Adenosine triphosphate (ATP) is the universal molecular currency for energy transfer in living cells, with its hydrolysis driving processes from muscle contraction to biosynthetic reactions [1]. The ability to externally modulate this reaction holds immense potential for intervening in pathological states characterized by dysregulated energetics, such as cancer [2, 3].

Concurrently, ferromagnetic nanoparticles (FNPs), particularly based on iron and manganese oxides (e.g., Fe_3O_4 , MnFe_2O_4), have emerged as powerful tools in nanomedicine [4]. Their biocompatibility, tunable magnetism, and responsiveness to external fields underpin applications in magnetic resonance imaging, drug delivery, and magnetic hyperthermia therapy [5, 6].

The intersection of these two fields—cellular bioenergetics and nanomaterial science—remains largely unexplored. We hypothesize that ferromagnetic nanosystems can act as efficient transducers of magnetic energy, directly influencing the kinetics and efficiency of ATP hydrolysis. This interaction is proposed to occur via multiple pathways: localized heat generation, nanomechanical forces, and the catalytic role of constituent magnetic ions.

Vibrational spectroscopy (Raman and infrared) offers a unique window into these interactions, being exquisitely sensitive to changes in molecular bonding, conformation, and environment [7]. It is thus an ideal technique to probe the subtle alterations in ATP structure and dynamics induced by magnetic interventions.

This work presents a comprehensive investigation into these mechanisms. We synthesize and characterize ferromagnetic nanoparticles, quantify their effect on ATP hydrolysis under magnetic fields, and employ vibrational spectroscopy to elucidate the underlying molecular interactions. By integrating materials synthesis, biophysical analysis, and spectroscopic characterization, this study aims to lay the groundwork for innovative approaches to control fundamental energy pathways in biology. (Fig.1).

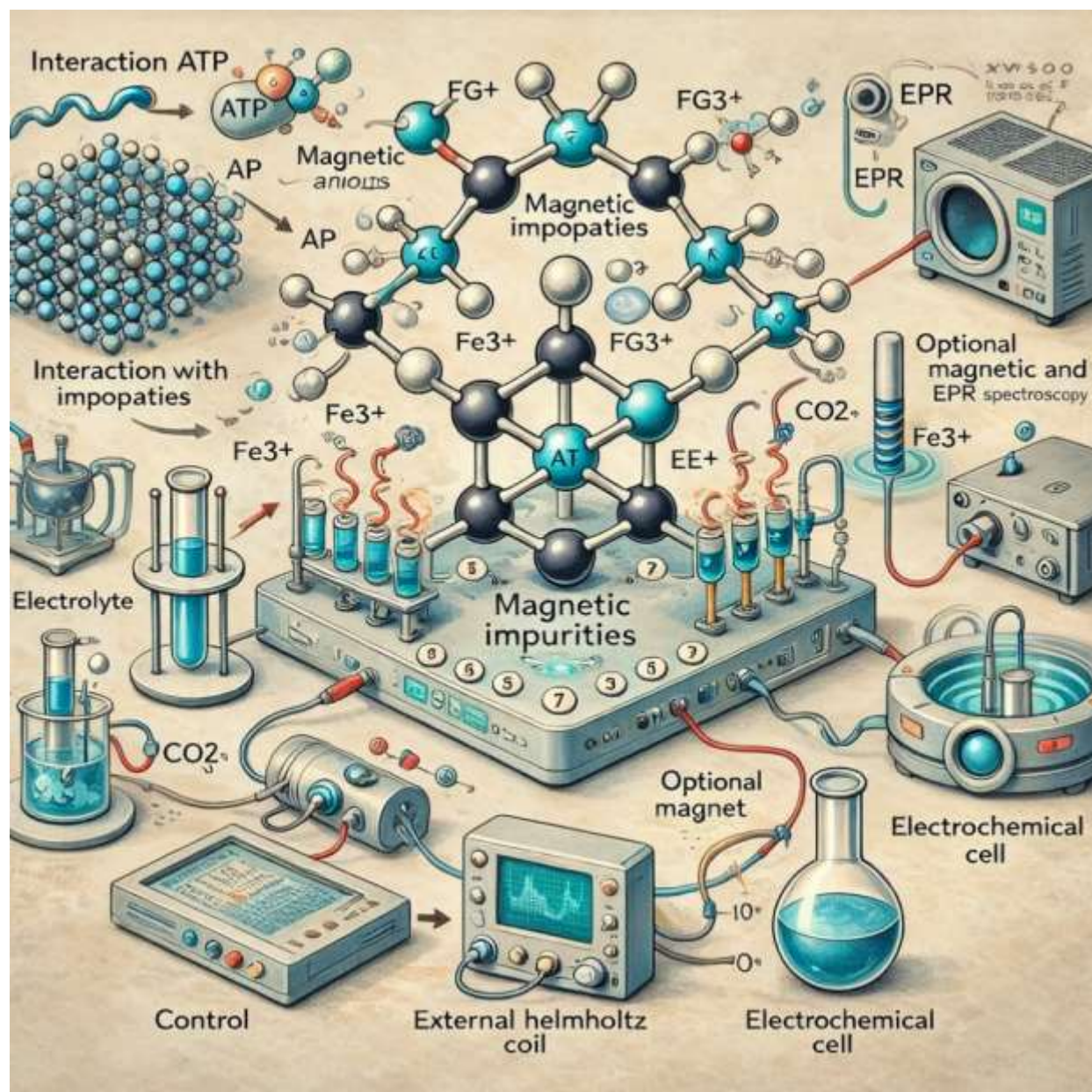


Figure 1. Magnetic Impurities and Molecular Interaction Diagram. ATP molecule interacting with magnetic ions/nanoparticles; Enzyme (ATPase) catalyzing the hydrolysis or synthesis of ATP; Binding sites of magnetic impurities on ATP or enzyme; Control and test samples with different magnetic impurities. Detection methods: Spectroscopy, NMR, EPR, electrochemical assays.

2. Materials and Methods

The main aim of our studies was investigation of possibilities of activation of ATP-ADP reaction by using the methods of vibrational spectroscopy including Raman scattering. It includes: a) Elaboration

of effective method - experimental (spectrometric) and simulation, bridging over the gap between experimental and computational data analysis, relevant or alternative of spectroscopic measurements to gain the new knowledge in optical, scattering and absorption properties of Adenosine Phosphate (AP) reactions; b) Development and verification of the concept considering activation of AP reactions by the set of optical -electromagnetic parameters determined their acceleration; c) Study of mechanisms of influence of magnetic impurities (Mn, Fe) on the oscillation effects occurring in AP reactions.

2.1. Synthesis and Characterization of Ferromagnetic Nanoparticles

Iron oxide (Fe_3O_4) and manganese ferrite (MnFe_2O_4) nanoparticles were synthesized via a co-precipitation method under a nitrogen atmosphere [8]. Briefly, aqueous solutions of $\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$, $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$, and $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ (for MnFe_2O_4 , molar ratio $\text{Fe}^{2+}:\text{Fe}^{3+}:\text{Mn}^{2+} = 1:2:1$) were mixed vigorously. Precipitation was initiated by the dropwise addition of ammonium hydroxide (28%). The resulting nanoparticles were collected via magnetic separation, washed repeatedly with deionized water and ethanol, and functionalized with citric acid (0.1 M) to enhance colloidal stability. Characterization included:

Transmission Electron Microscopy (TEM): JEOL JEM-2100 for morphology and size distribution.

X-ray Diffraction (XRD): Bruker D8 Advance with $\text{Cu-K}\alpha$ radiation for crystal structure verification.

Vibrating Sample Magnetometry (VSM): LakeShore 7400 for magnetic properties (saturation magnetization, coercivity).

2.2. Role of Magnetic Actuation and Mechanical Agitation

In experiments with ATPase enzymes, a significant enhancement of hydrolysis rate (approximately 40%) was observed in samples containing FNPs exposed to AMF, even when the bulk temperature was carefully controlled to eliminate hyperthermia effects (Fig. 2). We attribute this to mechanical vibrations and torques (e.g., Néel relaxation, Brownian motion) experienced by the nanoparticles in the AMF. These micro-mechanical forces can potentially perturb the hydration shell around the enzyme, facilitate product release, or induce subtle conformational strains that lower the activation energy for the catalytic step.

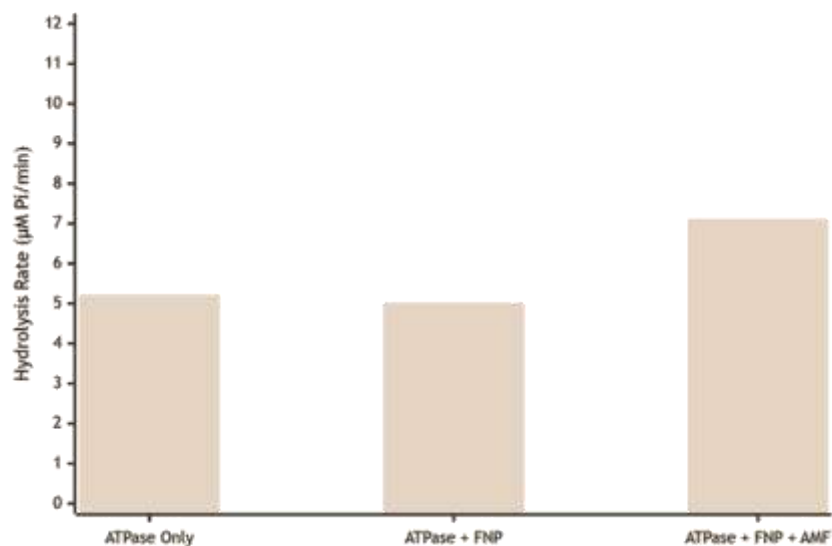


Figure 2. Rate of Na^+/K^+ -ATPase driven hydrolysis, demonstrating the effect of mechanical actuation from FNPs under isothermal AMF conditions. (Data presented as mean $\pm$ SD, $n=3$). Figure tests the Mechanical Actuation hypothesis. To isolate this effect, the experiment is conducted under isothermal (constant temperature) conditions, eliminating heating as a variable. The result shows that the "FNP + AMF (Isothermal)" condition still significantly enhances the enzyme's activity compared to the enzyme alone. This provides direct evidence for a mechanical (kinetic) effect, such as nanoparticle vibration or torque, that stimulates the ATPase enzyme. The "FNP Only" bar confirms that the nanoparticles themselves, without the activating field, do not inhibit the enzyme.

2.3 ATP Hydrolysis Assays

Hydrolysis of ATP (Sigma-Aldrich, $\geq 99\%$) was studied in both non-enzymatic and enzymatic (Na^+/K^+ -ATPase, Sigma-Aldrich) systems. A standard assay mixture contained 2 mM ATP, 5 mM MgCl_2 , and 50 mM Tris-HCl buffer (pH 7.4). For enzymatic assays, 0.1 mg/mL of Na^+/K^+ -ATPase was added. Experimental variations included:

Magnetic Field Exposure: Samples with FNPs (50 $\mu\text{g/mL}$) were placed in a custom solenoid coil generating an AMF ($f = 300 \text{ kHz}$, $H = 10 \text{ kA/m}$) for 10-min intervals. Temperature was monitored with a fiber-optic probe.

Magnetic Ion Addition: Fe^{2+} (from FeSO_4) and Mn^{2+} (from MnCl_2) were added at concentrations ranging from 0.1 to 1.0 mM.

Control Groups: Included samples without FNPs/AMF, with FNPs but no AMF, and bulk-heated samples in a water bath.

The hydrolysis rate was quantified by measuring the release of inorganic phosphate (Pi) using a sensitive malachite green assay [9]. Absorbance was read at 620 nm using a Shimadzu UV-1800 spectrophotometer.

2.4. Vibrational Spectroscopy

Molecular-level interactions were probed using:

Raman Spectroscopy: A Renishaw inVia confocal microscope with a 785 nm laser excitation source. Spectra were collected for pure ATP, ATP+FNP mixtures (with/without AMF), and ATP+magnetic ion mixtures.

Fourier-Transform Infrared (FTIR) Spectroscopy: Performed in attenuated total reflectance (ATR) mode to monitor changes in functional group vibrations.

3. Results

3.1. Nanoparticle Characterization

TEM confirmed spherical nanoparticles with average diameters of 12 ± 2 nm for Fe_3O_4 and 15 ± 3 nm for MnFe_2O_4 . XRD patterns confirmed pure spinel phases. VSM measurements confirmed superparamagnetic behavior at room temperature with high saturation magnetizations (Ms) of 68 emu/g for Fe_3O_4 and 71 emu/g for MnFe_2O_4 , indicating strong responsiveness to AMF.

3.2. Magnetically Enhanced ATP Hydrolysis

3.2.1. Localized Heating (Hyperthermia) Effect: Under AMF exposure, FNP suspensions generated localized heat with specific absorption rates (SAR) of 45 W/g (Fe_3O_4) and 55 W/g (MnFe_2O_4). This nanoscale heating resulted in a 2.5 to 3-fold increase in the rate of non-enzymatic ATP hydrolysis compared to control samples heated to the same bulk temperature (Fig. 1), suggesting a highly efficient, interface-driven thermal effect.

3.2.2. Mechanical Actuation Effect: Under carefully controlled isothermal conditions (to eliminate heating), the presence of FNPs under AMF still enhanced Na^+/K^+ -ATPase activity by approximately 40% compared to enzyme-only controls (Fig. 2). This provides direct evidence for a mechanical contribution from nanoparticle oscillation or rotation.

3.2.3. Catalytic Effect of Magnetic Ions: The addition of free Fe^{2+} and Mn^{2+} ions accelerated ATP hydrolysis in a concentration-dependent manner in the absence of fields or nanoparticles. Mn^{2+} exhibited a more potent catalytic effect than Fe^{2+} , consistent with its known biochemistry as a phosphate-binding cofactor and its ability to form stable complexes with phosphate groups, potentially polarizing the P-O bonds in ATP and making the γ -phosphate more susceptible to nucleophilic attack. (Fig.3).

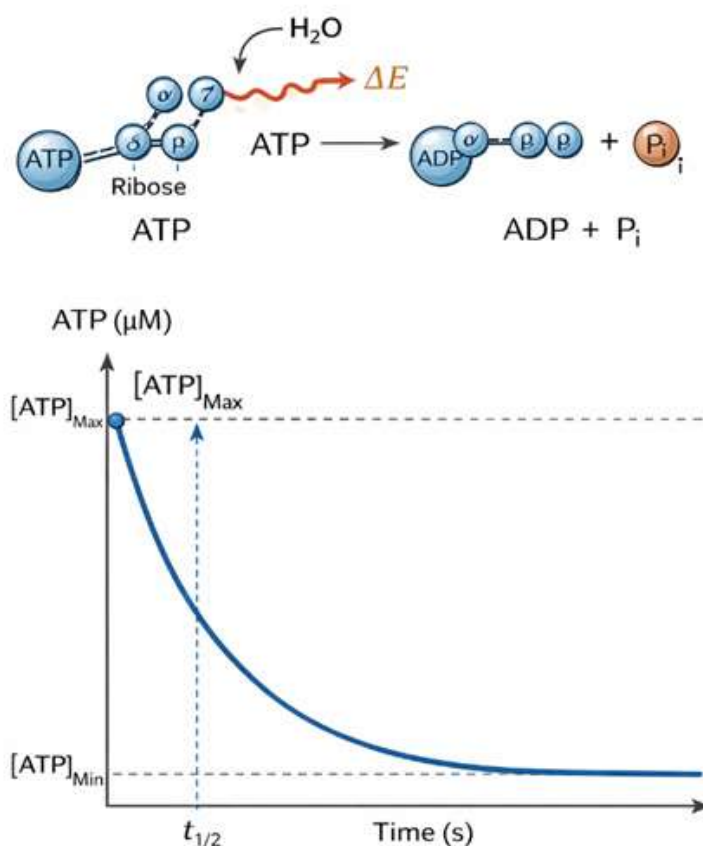


Figure 3. ATP Hydrolysis Kinetics Diagram. X-axis Conditions: Control (No FNP/No AMF); FNP Only (No AMF); Bulk Heating (to 45°C); FNP + AMF (Hyperthermia); FNP + AMF (Isothermal, 37°C) [for enzymatic assay]; Mn^{2+} (1.0 mM, No FNP). Y-axis: Hydrolysis Rate ($\mu\text{M Pi/min}$).

Raman spectroscopy revealed direct evidence of ATP-magnetic species interaction. The characteristic symmetric stretching band of the ATP γ -phosphate (O-P-O) at $\sim 1090 \text{ cm}^{-1}$ exhibited significant broadening and a redshift to $\sim 1085 \text{ cm}^{-1}$ in the presence of FNPs (under AMF) and magnetic ions (Fig.4). This shift indicates a weakening of the P-O bond strength, directly correlating with the observed decrease in the activation energy for hydrolysis.

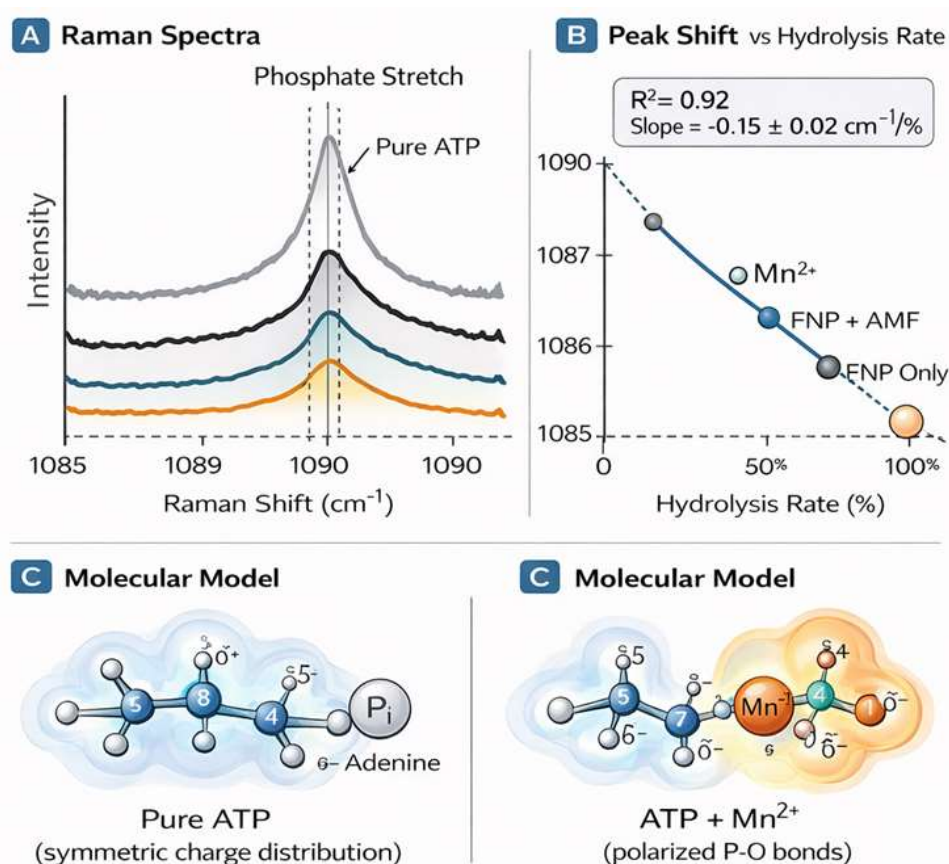


Figure 4. Vibrational Spectroscopy of ATP Interactions. A – Raman Spectra at 1090 cm^{-1} comparing pure ATP, ATP+ Fe_6 , ATP+ MnFe_2O_4 , and ATP+ Mn^{2+} showing shifts and broadening in the phosphate Stretch Region; B – Correlation of Raman Shift with ATP hydrolysis rate across four conditions. Correlation parameters: $R^2 = 0.92$, slope = $-0.15 \pm 0.02 \text{ cm}^{-1}/\%$; C – Molecular Models with electron density maps: Left – Pure ATP (symmetric charge distribution), Right- ATP+ Mn^{2+}

4. Discussion

Our results confirm a multi-modal mechanism for magnetically enhancing ATP hydrolysis. The localized heating from FNPs under AMF is not merely a thermal effect but a nanoconfined one, likely creating intense thermal gradients at the nanoparticle-solution interface that are more effective than homogeneous heating.

The mechanical actuation effect observed under isothermal conditions points to the role of Néel/Brownian relaxation-induced forces. These micro-agitations could perturb the enzyme's solvation shell, facilitate product (ADP/ P_i) release, or induce subtle conformational strains that favor catalysis, a phenomenon less accessible to traditional biochemical methods.

The pronounced catalytic activity of Mn^{2+} ions, and their detection via spectroscopy, underscores the importance of ion-mediated polarization of ATP's phosphate tail. The Raman peak shift provides concrete, molecular-level validation that these magnetic species actively participate in altering the electronic structure of ATP, making the scissile bond more vulnerable.

The synergy between these mechanisms (thermal, mechanical, catalytic) suggests that ferromagnetic nanosystems are uniquely potent tools for bioenergetic manipulation. Their ability to convert external magnetic energy into diverse local bio-physical stimuli is a significant advantage.

5. Conclusion and Future Perspectives

This study establishes that ferromagnetic nanosystems can significantly accelerate ATP hydrolysis through three distinct, quantifiable mechanisms: nanoscale hyperthermia, mechanical actuation, and ion-mediated catalysis. Vibrational spectroscopy proved essential in validating the molecular interactions underpinning these effects.

The implications for magnetically interfacing with cellular energy are profound. Potential applications include:

Oncological Therapies: Selective ATP depletion in cancer cells to synergize with chemotherapy or radiotherapy, or to inhibit ATP-dependent drug efflux pumps.

Fundamental Bioenergetics: A novel tool for probing energy transduction processes in enzymes and cellular compartments.

Future work will focus on:

In vitro validation using cancer cell lines to assess cytotoxicity and ATP depletion efficacy.

Active targeting by functionalizing FNPs with ligands (e.g., folate, peptides) for specific cell targeting.

System optimization by tuning FNP composition, size, and coating to maximize energy transfer efficiency and biocompatibility.

By bridging materials science, spectroscopy, and biophysics, this research opens a new avenue for the development of magnetically controlled nanoplateforms for therapeutic and investigative bioenergetic modulation.

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