2. Scientific accomplishments (max. 3 pages) – Results obtained during the reporting period.

1. __Study of the interaction of the laser beam with target by means of Finite Element Method__

The numerical study interaction of the laser beam with the target offers information on the impact of the laser parameters and target material characteristics on developing processes based on the phenomena indicated by the simulation results. For this purpose, finite element analysis is the method that fits best. There are two software variants that we have in mind, namely COMSOL and PIC. In a first stage, we used the COMSOL software to study the phenomena, processes and conditions obtained for the generation of ablation plasma, the Particle in cell (PIC) software being more suitable for the study of plasma movement and the particles that compose it, i.e. for the subsequent stage of study. Laser interaction with the silver target containing Fe and Ni impurities was numerically simulated and the results were used to explain the Experimental phenomena noticed on the thin films obtained by pulsed laser deposition technique. It resulted that the three instabilities, Plateau – Rayleigh instability (PRI), Rayleigh – Taylor instability (RTI), Richtmyer – Meshkov instability (RMI), and the “crown splash”, as phenomena related to fluids break-up are are responsible for the formation of droplets during the deposition of thin metal films. The explanation is based on the results obtained in COMSOL which indicates the formation of both the liquid phase and the gas and plasma during laser irradiation of the target. The fluid phase is highlighted by the point temperatures developed on the spot and in its immediate vicinity, over a distance until which the thermal diffusion takes place depending on the material characteristics.If the thermal energy developed on the spot that interacts with the laser radiation is also dependent on the laser parameters, as well as on the optical characteristics of the target material, the heat transfer on the surface of the material in the vicinity of the spot depends only on the thermal conductivity characteristics. Heat transfer in the target volume will be influenced by laser beam over a distance equal to the optical path (inverse of the absorption coefficient) and under the exponential attenuation effect given by the Beer-Lambert law, after which only the characteristics related to the thermal conductivity of the material will count. The same parameters for the numerical simulation and for the experimental proceedings were used: pulse energy of 100 mJ, 150 mJ and 180 mJ, 10 ns pulse width, 10 Hz pulse repetition and 168 μm spot radius and 10^{-2} Torr pressure in the deposition chamber. Parametric sweep was used to vary the pulse energy. The theory, mathematics and formulae to describe the physical phenomena and processes and their implementation in COMSOL simulation is as described in the articles previously published by our laboratory team [2, 3]. New conditions and extended geometry and domains have been added with this simulation to analyse and anticipate thermal behaviour and heat transfer when plasma of ablation travels from the target to the substrate and the new model was published by our laboratory [1]. The geometry includes the target and the environment surrounding the target in the deposition chamber, as well as the non-homogeneous material of the target (Figure 1) [1].

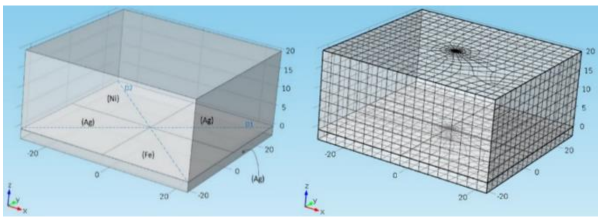

Figure 1. Geometry with materials and mesh for COMSOL simulation [1]. The results are collected in the nodes as per the mesh which is set-up as “extremely fine” for the areas of interest and “coarse” for the rest of geometry in order to optimize the data accuracy versus computing time. The acquired data are used to obtain phase change diagrams T (d) on the target in spot and its vicinity, as much as heating takes place.

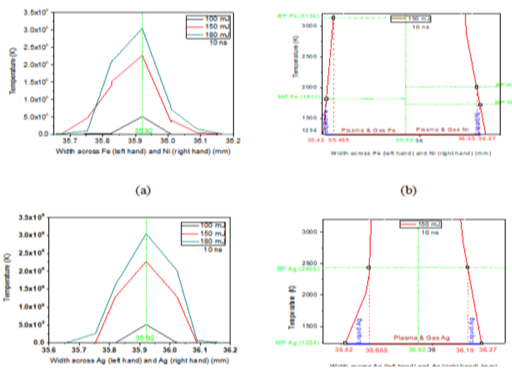

Figure 2. Phase change diagrams T (d) on the target irradiated surface after 10 ns for: iron and nickel at different energies (a) and their co-existing phases at 150 mJ (b); silver at different energies (c) and its co-existing phases at 150 mJ (d) [1]

The silver melting and boiling points, as well as those of the impurities of iron and nickel are used as reference for phase change in the diagrams. Phase components are analyzed in the diagrams of Figure 3 [1]. The thermal effects in the deposition chamber were analyzed by isosurface diagrams and 2 D plots as presented in Figure 4 and Figure 5, respectively.

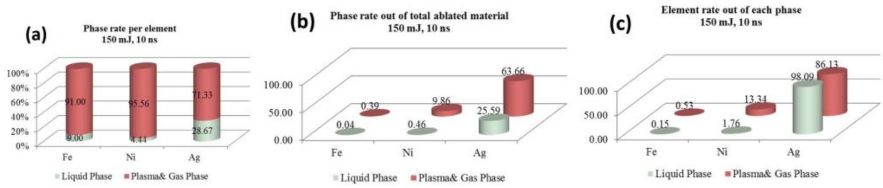

Figure 3. Study of phases fractions during ablation, for t = τ = 10 ns, based on COMSOL simulation. (a) Phase rate per element developed during laser ablation at 150 mJ on COMSOL simulation; (b) Phase rate out of total ablated material based on COMSOL simulation; (c) Element rate out of each phase during ablation to different energies based on COMSOL simulation [1]

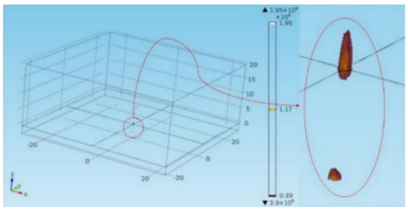

Figure 4. 3D Plot representing the Isosurface where heating is high enough to favor the plasma formation on the target and heat transfer in the surrounding environment [1]

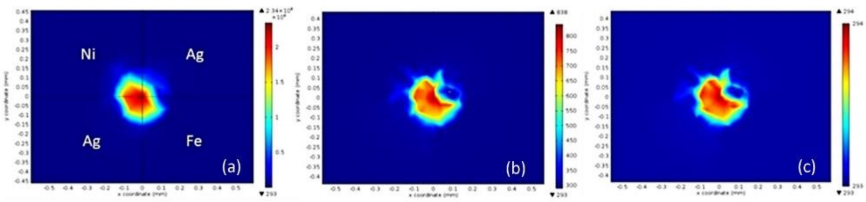

Figure 5. 2D Heating plots in xOy plane at 10 ns when using 150 mJ laser energy: a) on the target surface; b) at 10 mm height from target; c) at 20 mm height from target [1]

Conditions for existence of different phases of ablated material in the deposition chamber on the plasma plume trajectory are analyzed in phase diagrams as in Figure 6.

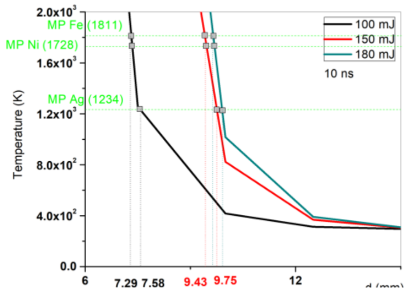

Figure 6. Thermal effects in the deposition chamber target surrounding atmosphere in (x, y, z) = (0, 0, z) and z Є [0, d] and d=20 mm (distance between target and support) [1]

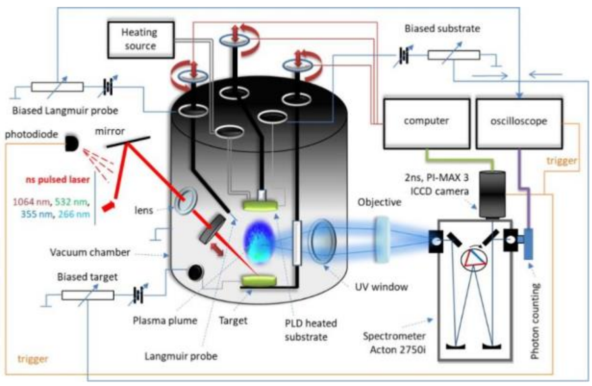

Figure 7. Experimental installation for PLD and LIBS in Atmosphere Optics, Spectroscopy and Lasers Laboratory (http://spectroscopy.phys.uaic.ro)

The fluid phases developed due to thermal effects during laser interaction with the target material explain droplets formation in terms of instabilities of PRI, RTI and RMI type, as well as crown splash fluid break-up at the impact with the solid substrate or still melted film on the substrate. Thin film deposition for experimental study to compare with simulation results was conducted on the installation presented in Figure 7. The laser system used was YG981E/IR- 10 Hz, and the parameters: τ=10 ns pulse width, λ=532 nm wavelength, α=45° incident angle and ν = 10 Hz pulse repetition time (Figure 1). The pressure in the deposition chamber was $3 \cdot 10^{-2}$ Torr. The SEM images of figure 7 evidence different shapes of droplets, each being specific to a certain pulse energy of the laser beam in interaction with the silver target doped with Fe and Ni impurities, and that corresponds to certain amounts (percentage) of liquid, gas or plasma in the total fluid phase, each being susceptible to one or another of the fluid break-up instabilities.

“These instabilities are based on the induced perturbing phenomena such as electromagnetic field of laser beam for the first 10 ns, the electric field of the diffusion current generated by the charged carriers (ions in plasma) during their motion and the phase states developed during ablation and evidenced in the numerical simulation in COMSOL” [1]. Crown splash effect is noticed for high energy of 180 mJ (Figure 7 a) and b) while pearl shaped droplets are noticed for lower pulse energy (100 mJ). Study of the influence of each fluid-break-up phenomena and instabilities will provide with information and answers for finding solutions to diminish and avoid droplets formation or or on the contrary, to control their size and shape when they are aimed to be obtained.

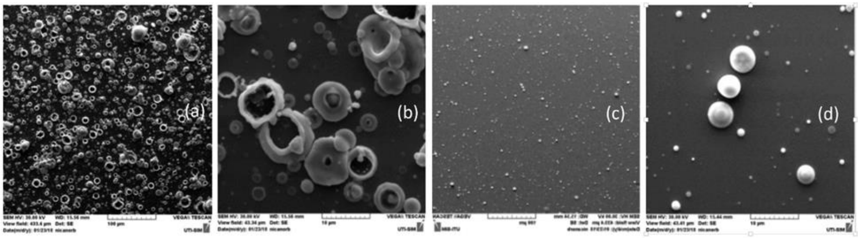

Figure 7. Compared SEM images of droplets on the thin films A (180 mJ) and B (100 mJ): (a) Sample A (180 mJ) 500x; (b) Sample A (180 mJ) 5kx; (c) Sample B (100 mJ) 500x; (d) Sample B (100 mJ) 5kx [1]

2. Numerical study of CdO/Se and CdS/Se dual targets to synthesis CdSe nanoparticles on glass slab or other supports by PLD technique

Modeling and simulation of physical and chemical phenomena has an important role in obtaining information leading to a reduction in the number of experimental trials. In this sense, for the preparation of the conditions for deposition with pulsed laser of some quantum dots of cadmium selenide (CdSe), the study of the fulfillment of the ablation conditions of the precursor materials was performed with finite element method, using COMSOL analytical software platform. The method of pulsed laser deposition (PLD) of thin layers and obtaining nanoparticles represents the prospect of developing clean, ecofriendly technologies. Irradiation of the dual targets in the ablation and PLD process is studied for 532 nm laser beam wavelength, 150 mJ energy on a spot of 0.650 mm, pulse width of 10 ns and 10 Hz frequency. Ablation is studied according to the phase diagrams obtained as a result of modeling and simulation in COMSOL, in terms of temperatures relative to boiling points which represent the vaporization temperature (boiling point) in the case of Se and sublimation and decomposition in the case of CdO and CdS.

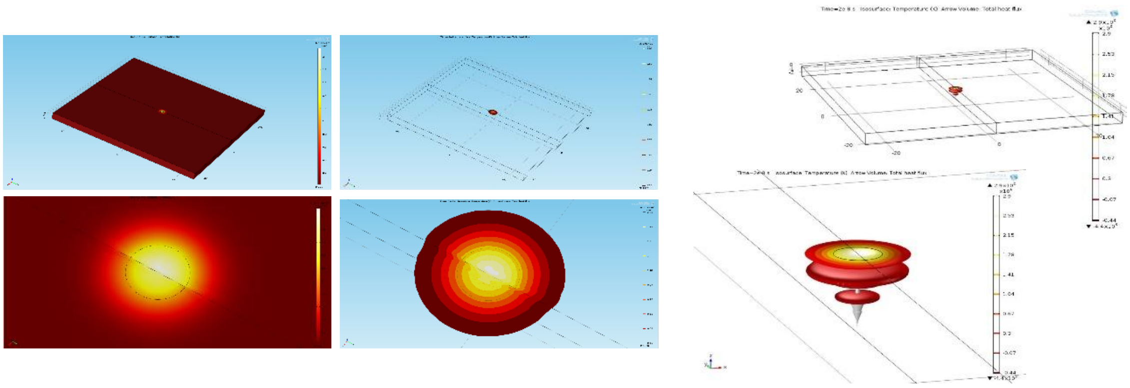

Figure 1. a) Thermal effect on target surface with zoom on spot b)Isosurface thermal effects at pulse width (10 ns) in the target with zoom on spot, c) Isosurface thermal effects at pulse width (20 ns) in the target with zoom on spot

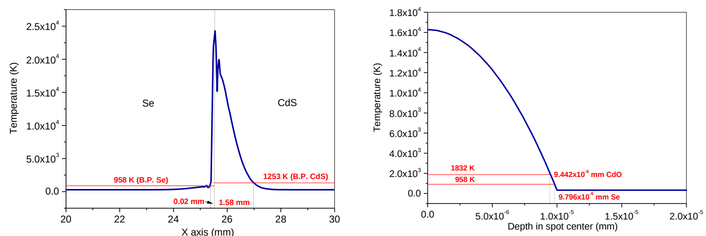

Figure 2. Phase diagrams under different cut lines in pulse width

The ablation compared efficiency is also observed from the phase diagrams in which the temperature is represented in time and when it is observed that from the 20 ns how much the heating of the irradiated spot takes place under the action of the 10 ns pulse. It follows from the simulation that reaching the boiling points is more efficient for the dual target CdO / Se compared to the dual target CdS / Se. The results are presented in phase diagrams and plots in the Figures 1. Irradiation of the dual targets in the ablation and PLD process is studied for 532 nm laser beam wavelength, 150 mJ energy on a spot of 0.650 mm, pulse width of 10 ns and 10 Hz frequency (Figures 2). The ablation compared efficiency is also observed from the phase diagrams in which the temperature is represented in time and when it is observed that from the 20 ns how much the heating of the irradiated spot takes place under the action of the 10 ns pulse. It follows from the simulation that reaching the boiling points is more efficient for the dual target CdO / Se compared to the dual target CdS / Se. The simulation in COMSOL, however, predicts that only CdO has the necessary properties to interact with laser radiation efficiently and in the presence of selenium.

References:
[1]Cocean, I. Cocean, S. Gurlui, F. Iacomi, Study of the pulsed laser deposition phenomena by means of Comsol Multiphysics, U.P.B. Sci. Bull., Series A, Vol. 79, Iss. 2, 2017, [2, 3] Lide, D.R. CRC Handbook of Chemistry and Physics 88TH Edition 2007-2008. CRC Press, Taylor & Francis, Boca Raton, FL 2007, p. 4-86 & p. 4-54

3. Group members (table):

- List each member, his/her role in project and the Full Time Equivalent (FTE) time in project. The FTE formula to be used is: FTE = Total number of worked hours /Total number of hours per reporting period[1];
- List PhD/Master students and current position/job in the institution.

Table of group members

No.	Name and surname	Role in the project	Full Time Equivalent (FTE)
1	Gurlui Silviu	Project Director	
2	Dimitriu Dan-Gheorghe	Team member	
3	Cimpoeșu Nicanor	Team member	
4	Cocean Iuliana	Team member	
5	Cocean Alexandru	Team member	
6	Bulai Georgiana	Team member	
7	Lina Diana	Financial responsible	
8	Iacob Silvia	Team member	
9	Postolachi Cristina	Team member	

Table of PhD/Master students

No.	Name and surname	PhD/Master student	Position/job in the institution
1	Lina Diana	PhD	Financial administrator
2	Iacob Silvia	PhD	Research assistant
3	Postolachi Cristina	PhD	None

4. Deliverables in the last year related to the project:

ISI Papers:

[1]. Cocean, A., Cocean, I., Cocean, G., Postolachi, C., Pricop, D.A., Munteanu, B.S., Cimpoesu, N., Gurlui, S., Study of physico-chemical interactions during the production of silver citrate nanocomposites with hemp fiber, (2021), Nanomaterials, 11 (10), art. no. 2560

[2]. Cocean, A., Cocean, I., Cimpoesu, N., Cocean, G., Cimpoesu, R., Postolachi, C., Popescu, V., Gurlui, S., Laser induced method to produce curcuminoid-silanol thin films for

[1] Total number of hours (for a certain period) = 170 average monthly hours x number of months (e.g., for a full year: 170 hours/month x 12 months = 2040 hours)

transdermal patches using irradiation of turmeric target, (2021) Applied Sciences (Switzerland), 11 (9), art. no. 4030

[3]. Cocean, A., Cocean, I., Gurlu, S., Influence of the impurities to the composite materials in laser ablation phenomena, (2021), UPB Scientific Bulletin, Series A: Applied Mathematics and Physics, 83 (3), pp. 225-238

[4]. Kadri, L., Bulai, G., Carlescu, A., George, S., Gurlui, S., Leontie, L., Doroftei, C., Adnane, M., Effect of target sintering temperature on the morphological and optical properties of pulsed laser deposited TiO2 thin films, (2021), Coatings, 11 (5), art. no. 561

[5]. Catalin Panaghie, Ramona Cimpoesu, Bogdan Istrate, Nicanor Cimpoesu, Mihai-Adrian Bernevig, Georgeta Zegan, Ana-Maria Roman, Romeu Chelariu and Alina Sodor, New Zn3Mg-xY Alloys: Characteristics, Microstructural Evolution and Corrosion Behavior, Materials 2021, 14, 2505. https://doi.org/10.3390/ma14102505

Conferences

[1]. Alexandru COCEAN , Iuliana COCEAN, Georgiana BULAI, Cristina POSTOLACHI, Bogdan MUNTEANU, Nicanor CIMPOESU, Silviu GURLUI, Invited Conference, Trace elements Photo-Analysis for environmental applications: a case study, The 3rd International Workshop Advances on Photocatalysis including Environmental and Energy Applications AdvPhotoCat-EE 2021, June 28-29, 2021

[2]. Alexandru COCEAN, Dorin BOTOC, Monica SIROUX, Cristina POSTOLACHI, Iuliana COCEAN, Silviu GURLUI, AMC-COMSOL: the new finite element technique to increase solar cell conversion, The 3rd International Workshop Advances on Photocatalysis including Environmental and Energy Applications AdvPhotoCat-EE 2021, June 28-29, 2021

[3]. Cristina POSTOLACHI, Mirela SUCHEA, Ioan-Valentin TUDOSE, Alexandru COCEAN, Iuliana COCEAN, Bogdanel Silvestru MUNTEANU, Nicanor CIMPOESU and Silviu GURLUI, Quantum Dots Pulsed Laser Deposition – a new simulation technique, The 3rd International Workshop Advances on Photocatalysis including Environmental and Energy Applications AdvPhotoCat-EE 2021, June 28-29, 2021

[4]. Iuliana COCEAN, Alexandru COCEAN, Cristina POSTOLACHI, Bogdanel Silvestru MUNTEANU, Nicanor CIMPOESU and Silviu GURLUI, High pulsed-laser effect on the hemp composite – advanced materials, The 3rd International Workshop Advances on Photocatalysis including Environmental and Energy Applications AdvPhotoCat-EE 2021, June 28-29, 2021

[5]. Silviu GURLUI, Alexandru COCEAN, Cristina POSTOLACHI, Georgiana COCEAN Iuliana COCEAN, Light interaction, pollution and SARS-Cov2: protection Mask biocompatibility-overview, The 3rd International Workshop Advances on Photocatalysis including Environmental and Energy Applications AdvPhotoCat-EE 2021, June 28-29, 2021

[6]. Alexandru COCEAN, Iuliana COCEAN, Cristina POSTOLACHI, Georgiana COCEAN and Silviu GURLUI, Laser induced chitin deacetylation- cutting-edge technology for “natural biological waste, The 3rd International Workshop Advances on Photocatalysis including Environmental and Energy Applications AdvPhotoCat-EE 2021, June 28-29, 2021

[7]. Cristina POSTOLACHI, Mirela SUCHEA, Ioan-Valentin TUDOSE, Alexandru COCEAN, Iuliana COCEAN, Bogdanel Silvestru MUNTEANU, Nicanor CIMPOESU and Silviu GURLUI, CdSe Quantum Dots insertion effect on the alpha-keratin PLD-thin films, The 3rd International Workshop Advances on Photocatalysis including Environmental and Energy Applications AdvPhotoCat-EE 2021, June 28-29, 2021

[8]. A. Cocean, I. Cocean, G. Cocean, C. Postolachi, B. Munteanu, N. Cimpoesu, S. Gurlui, Keratin-based polymer nanofilm membranes for medical applications, 13th International Conference on Physics of Advanced Materials (ICPAM-13), September 24 – 30, 2021, at the Hotel Eden Roc by Brava Hoteles, Sant Feliu de Guixols, Costa Brava, Spain
[9]. C. Postolachi, A. Cocean, I. Cocean, G. Cocean, B. Munteanu, N. Cimpoesu, S. Gurlui,Study of Si/SiO2 core/shell Quantum Dots produced by Pulsed Laser Deposition, 13th International Conference on Physics of Advanced Materials (ICPAM-13), September 24 – 30, 2021, at the Hotel Eden Roc by Brava Hoteles, Sant Feliu de Guixols, Costa Brava, Spain

5. Further group activities (max. 1 page):

- Collaborations, education, outreach.

The following activities will consider both round tables with partners in Germany but also with other partners in Austria, Bucharest or France to achieve the proposed equipment and targets. Both doctoral students and those with a master's or bachelor's degree who have research topics in this field of laser and energy particle physics will be trained.

The following research topics will be developed

1. Performing PIC codes (using FAIR infrastructure) to investigate the interaction & simulation hydrodynamic expansion (FAIR)
2. Making prototype targets on standard laser target holders used at FAIR and characterize them by means: space-time resolved optical emission spectroscopy, UV-VIS/FTIR spectroscopy, XRD, XPS, AFM, scanning electron microscopy SEM/ EDX/EDS (at LOASL)
3. Study of PLD thin films doped with nanoparticles - Designed and manufacture the of the new-KIT-Vacuum simulation chamber for transport, making and analyzing special PLD thin films dedicated to FAIR / APPA / MML / Plasma Physics / PHELIX experiments. Enhanced vacuum transport beamline for the laser at FAIR
4. Study of the interaction of the PHELIX laser beam with targets by means of Particle in Cell (PIC)-simulation computer techniques

6. Financial Report (budget usage) for the reporting period (see the Annex).

7. Research plan and goals for the next year (max. 1 page).

Study of the doped targets under high power laser beam (PHELIX). Experiments.

1. Designed and manufacture the of the new-KIT-Vacuum simulation chamber for transport, making and analyzing special PLD thin films dedicated to FAIR / APPA / MML / Plasma Physics / PHELIX experiments. Enhanced vacuum transport beamline for the laser at FAIR
2. Study of the interaction of the PHELIX laser beam with targets by means of Particle in Cell (PIC)- simulation computer techniques