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PROGRAM & ABSTRACTS

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Structure and Expansion of a Plume Emitted During Laser Ablation of Multi-Component Materials.

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Pulsed laser deposition is a method frequently used for creating thin films of various materials on solid substrates. High energy laser pulse causes evaporation of the target material, forming a plume which subsequently expands and moves with high speed from the target. Thin film of the evaporated material is deposited on the substrate placed at some distance in front of the target. The behavior of the plume influences both the stoichiometry and homogeneity of the deposited layer – the final product of the process. Better understanding of the process of expansion of the plume, variation of its structure as well as deposition of the material itself is therefore very important and should give us opportunity for better control of formation of the deposited layer.

Laser deposition process is very fast and very hard to observe. Changes of the plume structure cannot be observed in detail experimentally; it is particularly difficult in the case of multicomponent materials consisting of molecules with disparate masses which expand with different velocities. To overcome that, we performed numerical calculations of the phenomenon using the Direct Simulation Monte Carlo method.

The present paper is a continuation of our previous work on the expansion of the plume of hydroxyapatite [1] and carbon (the last one obtained from a graphite target) [2].

Hydroxyapatite is a multicomponent, biocompatible material used in medical prosthetics. The plume of hydroxyapatite consists of four components (Ca, P, O, H) with different molecular masses. The expansion of the hydroxyapatite plume was investigated experimentally and numerically in our laboratory. It was found, that if the plume expanded into an ambient gas – water vapour – the quality of obtained layers was much better than for expansion into vacuum.

Investigation of the expansion of carbon plume into vacuum and into nitrogen ambient gas confirmed the result, that presence of some ambient gas may improve the quality of the deposited layer – also in the case of one component plume.

In both investigated cases, when the ambient gas was present, two shock waves could be observed: the external wave in the ambient gas in front of the moving plume („bow shock") and the internal wave, in the plume itself, moving backwards from the front to the rear side of the plume (Fig. 1).

In the present work we investigate the external and internal shocks described above and also the third shock generated when the plume collides with the substrate. This shock may be generated in both cases – expansion into vacuum and into an ambient gas, provided that part of the material of the plume is reflected from the substrate and not deposited on it. The target from which the plume is evaporated is made out of tungsten tetraboride (WB4), so the plume consists of two disparate mass components – tungsten and boron [3]. The plume is evaporated into vacuum (Fig. 2) and into an ambient gas, argon.

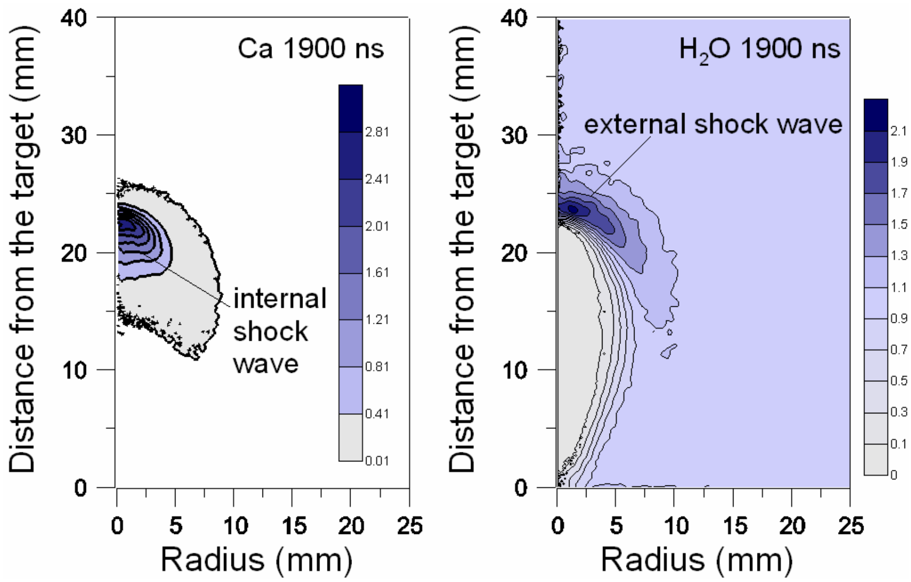

Fig. 1. Internal and external shock waves in the process of expansion of hydroxyapatite in water vapour [1].

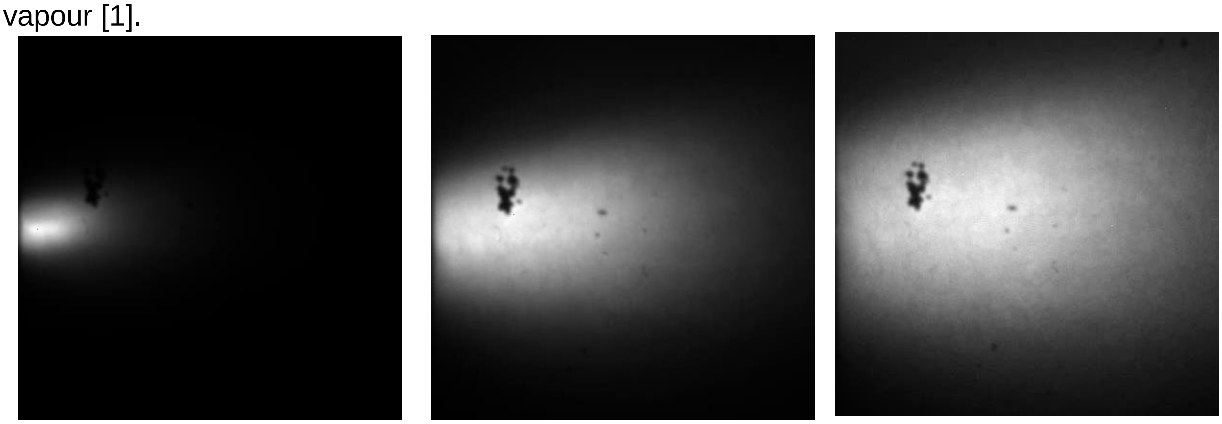

Fig. 2. Expansion of the tungsten tetraboride plume in vacuum. From the left: t=400ns, 1200ns and 2000ns after the laser pulse.

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References:

1. Słowicka A.M., Walenta Z.A., Szymański Z., Expansion of a multi-component laser-ablated plume, EUROPEAN PHYSICAL JOURNAL-APPLIED PHYSICS, 56, 11101-p1-8, 2011

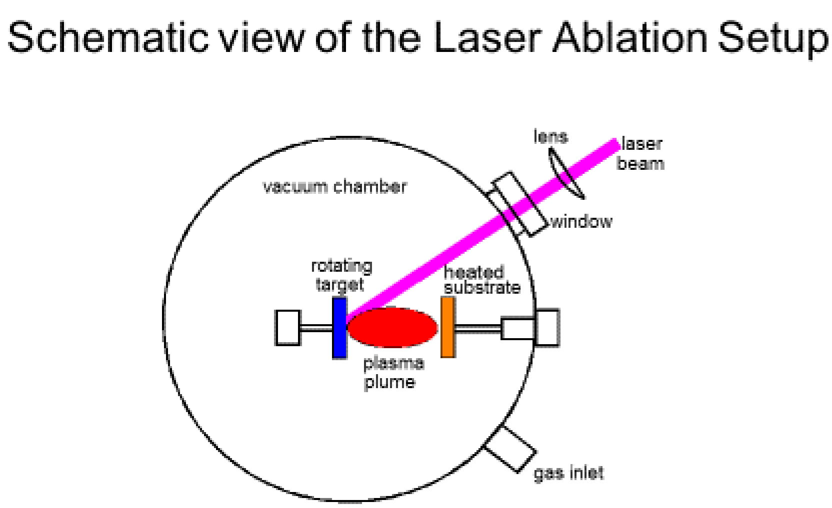
2. Słowicka A.M., Walenta Z.A., Szymański Z., Structure of the plume emitted during laser ablation of materials, Proceedings of 28th International Symposium on Shock Waves, Editor: K. Kontis, Heidelberg: Springer, 777-782, 2012

3. Mościcki T., Expansion of laser-ablated two-component plume with disparate masses, PHYSICA SCRIPTA, T161, 014024,1-4, 2014

Presentation

1)

2)

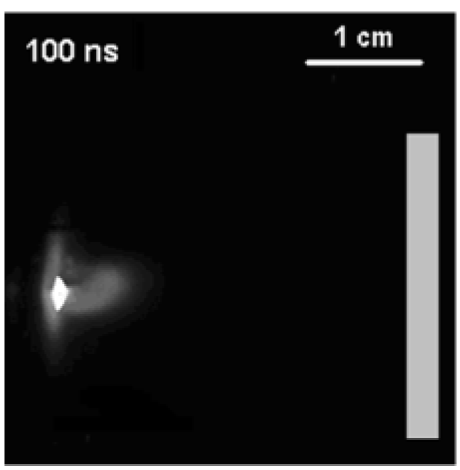


3)

Our aim - better understanding the phenomena, which occur in the expanding plume, as they may influence the quality of deposited layers.

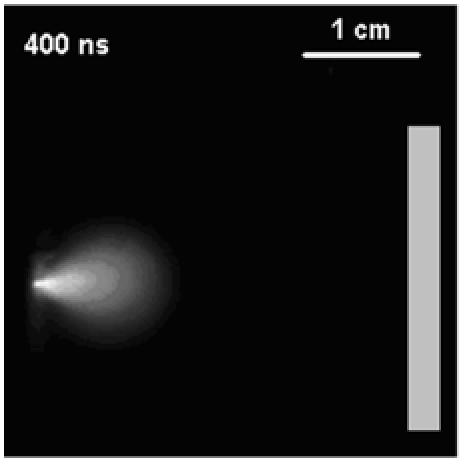
4)

Experiment – expansion of the HA-plasma
(hydroxyapatite $Ca_{10}(PO_4)_6(OH)_2$)
into air at p=0.008 Pa (nearly vacuum)



5)

Experiment – expansion of the HA-plasma into water vapour at p=18 Pa



6)

The expansion of the plume is described with the use of Direct Simulation Monte Carlo (DSMC) technique..

Specific assumptions:

- Outflowing medium consists of single atoms of Tungsten and Boron.
- Total number of emitted „representative" atoms in the range $10^6 - 10^7$ (which corresponds to the number of real atoms about $5 \cdot 10^{15}$)
- Boron and Tungsten outflow into vacuum
- Tungsten tetraboride WB_4 outflows into vacuum and into atmosphere of Nitrogen gas at pressure of 20 pascals

7)

100-400 ns after beginning of the laser pulse the particle velocity distribution in the cloud is „shifted Maxwellian":

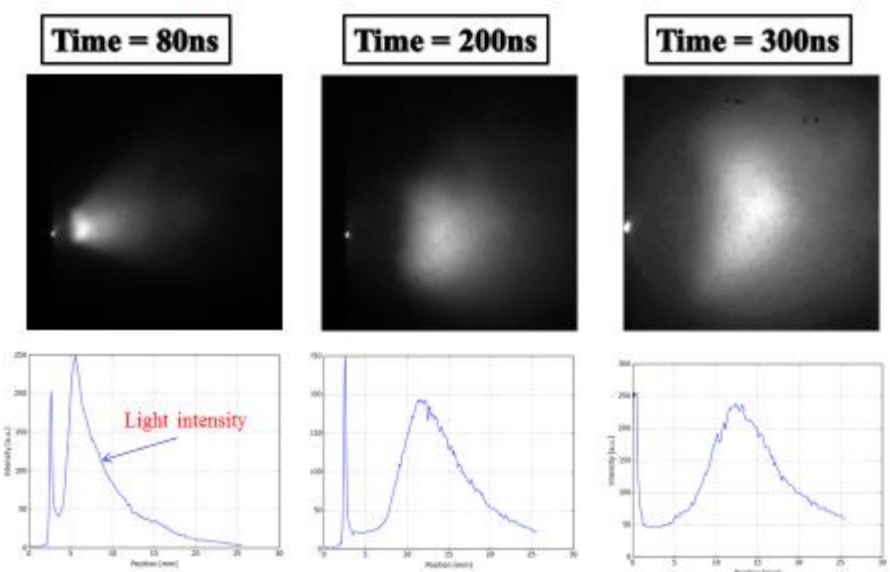
$$f(t) = C_0 \exp\left(-\frac{m}{2k_B T_{xy}} \left(v_x^2 + v_y^2 \right) - \frac{m}{2k_B T_z} \left(v_z - v_0 \right)^2 \right)$$

where:

m	- particle mass
v_x, v_y, v_z	- components of thermal velocity of a particle
v_0	- mass flow velocity perpendicular to the surface
T_{xy}	- „perpendicular" temperature
T_z	- „parallel" temperature
k_B	- Boltzmann constant

8)

Experimental results for Boron



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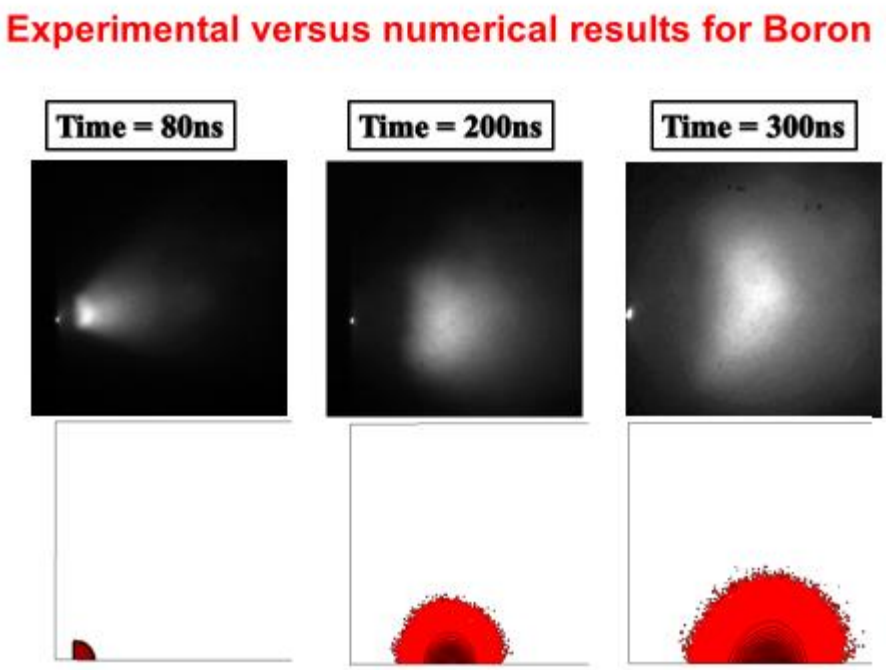
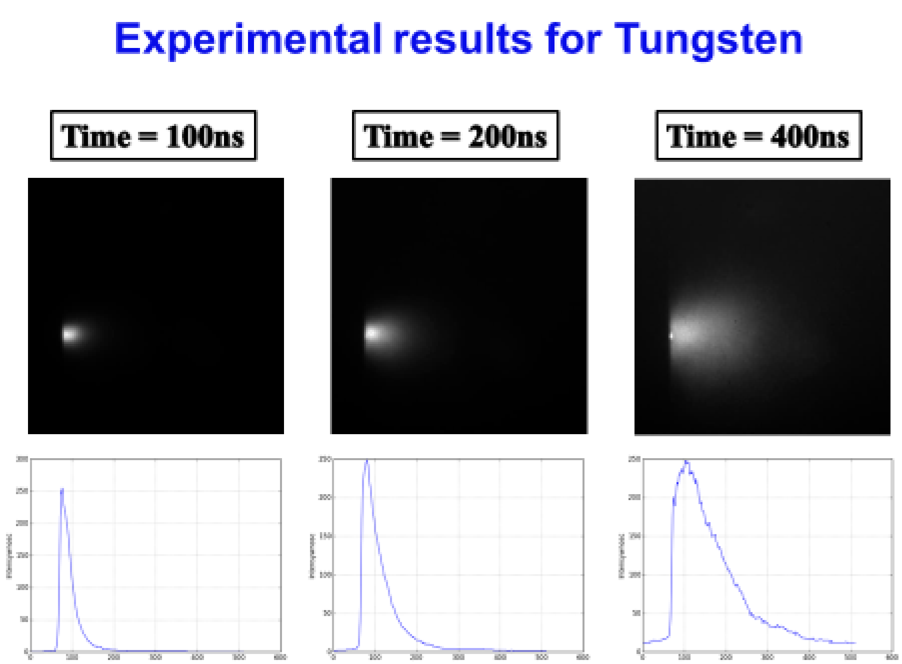
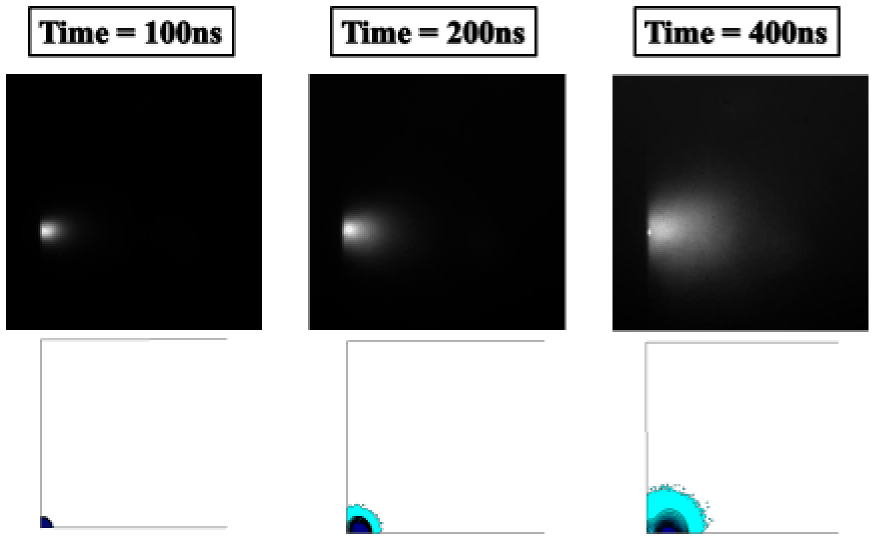

Experimental versus numerical results for Boron
Time = 80ns
Time = 200ns
Time = 300ns

10)


Experimental results for Tungsten
Time = 100ns
Time = 200ns
Time = 400ns

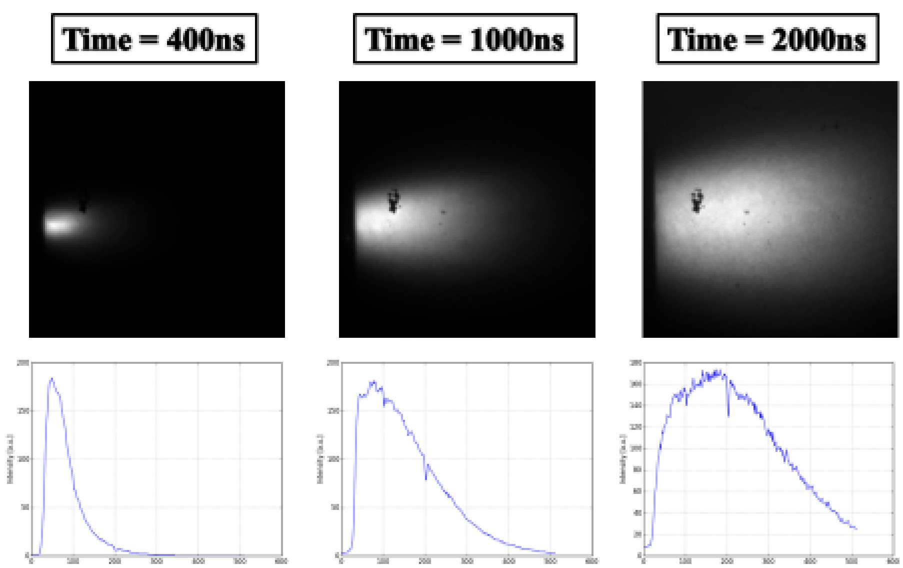
11)

Experimental versus numerical results for Tungsten



12)

Experimental results for WB_4 in vacuum



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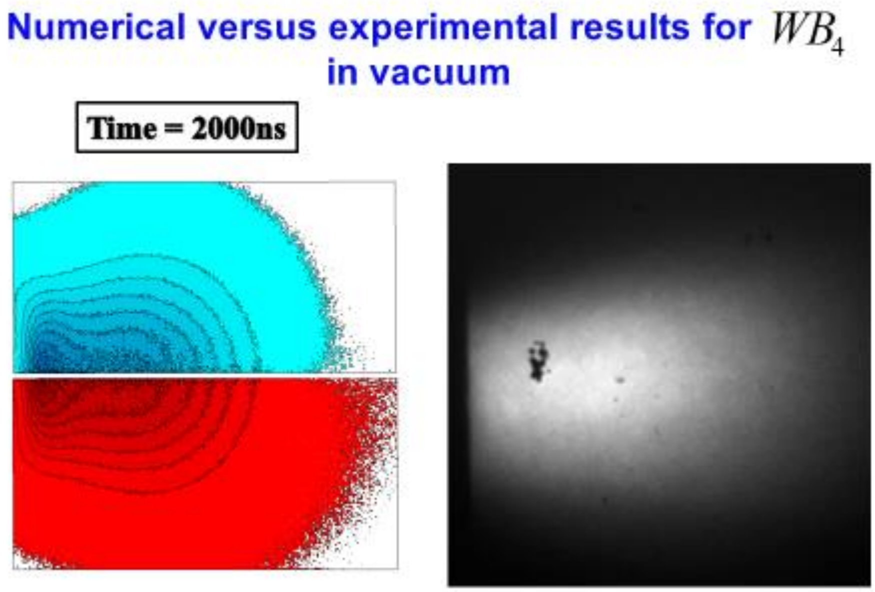
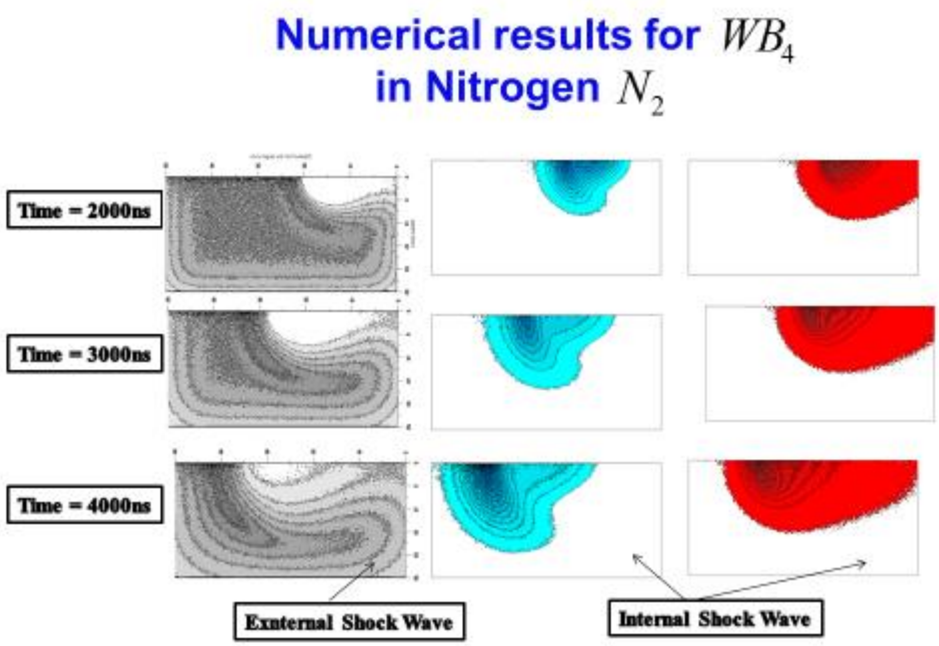
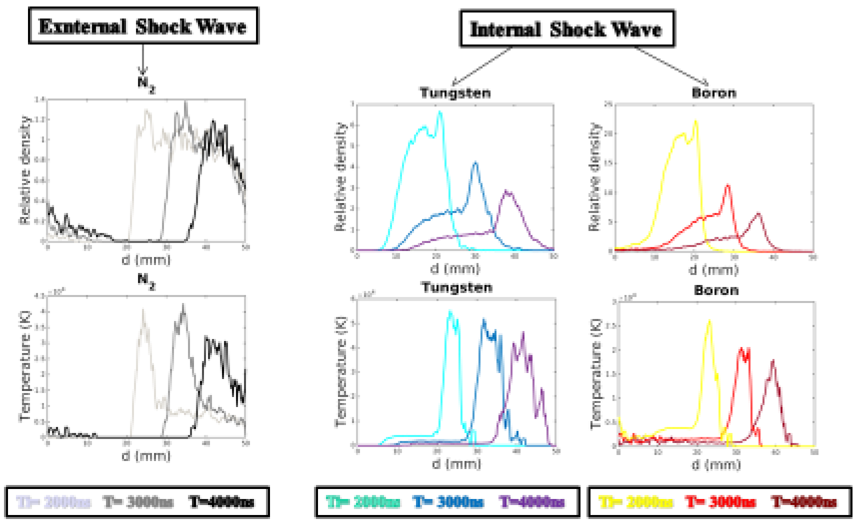

Numerical versus experimental results for WB_4 in vacuum
Time = 2000ns

14)


Numerical results for WB_4 in Nitrogen N_2
Time = 2000ns
Time = 3000ns
Time = 4000ns
Exnternal Shock Wave
Internal Shock Wave

15)

Numerical results for WB_4 in Nitrogen N_2



16)

CONCLUSIONS:

1. THE DIRECT MONTE CARLO SIMULATION METHOD SEEMS ADEQUATE FOR SIMULATION OF THE PLUME BEHAVIOUR DURING THE PULSED LASER DEPOSITION OF THIN FILMS.

2. BEHAVIOUR OF TUNGSTEN TETRABORIDE WB_4 SEEMS TO BE SIMILAR TO THAT OF HYDROXYAPATITE, IN SPITE OF VERY LARGE DIFFERENCE OF MOLECULAR MASSES OF TUNGSTEN (183.84) AND BORON (10.8).

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