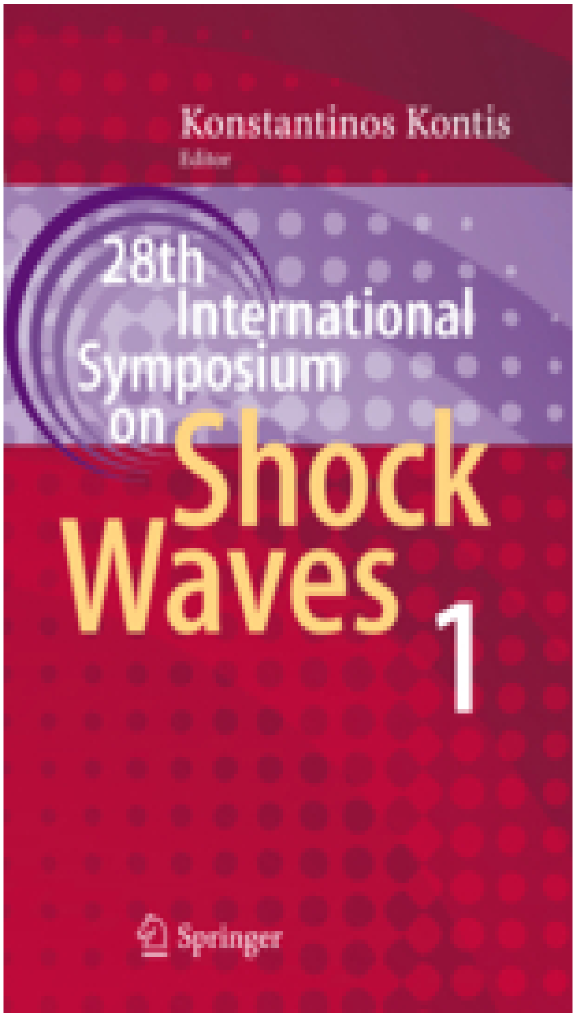

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Structure of the plume emitted during laser ablation of materials

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1 Introduction

Laser ablation is a frequently used method of removing material from a solid surface by irradiating it with a powerful laser beam. It may be applied to machining materials, cleaning contaminated surfaces, deposition of thin coatings on surfaces etc. High energy, short duration laser pulse, focused on a small area of the target surface heats and evaporates it, forming a thin layer of very dense plasma. The plasma layer may further absorb energy from the laser radiation, which increases its temperature and pressure. Subsequent expansion of this hot, high pressure layer of plasma leads to its acceleration in the direction perpendicular to the surface, and finally, to formation of the plume of approximately spherical shape, moving outwards from the target with high speed. The behaviour of the plume may influence the quality of the deposited layer, which is important if deposition is the goal of the process. This is particularly the case if the deposited material consists of disparate mass components. The light components move faster than the heavy ones and tend to spread on larger area of the substrate. In consequence the stoichiometry of the deposited material is not preserved. To improve the situation, the deposition process may be performed in the atmosphere of an ambient gas, which decelerates both the motion of the plume as a whole and its expansion. Deceleration is stronger for light components of the plume, which makes the expanding plume more uniform.

2 Model of expansion of the plume into ambient gas

When the plume moves through the ambient gas with supersonic speed, the bow shock (”external shock”) is formed in front of it. The increased pressure behind this

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shock acts on the front side of the plume decelerating it and generating a backwards oriented compression wave in the plume itself. This compression eventually transforms into a backward facing shock wave (”internal shock”). The gas from the rear part of the plume, moving faster than the front, passes through the internal shock, being compressed and decelerated, and joins the slower moving front. All that time the internal shock moves backward with respect to the centre of mass of the plume and may disappear after reaching its rear border. This is the case if the speed of the motion of the plume is high enough to produce vacuum behind it. No wave reflection from vacuum may take place. The model of the plume expansion with the external and internal shocks has been adopted from the spherically symmetric model of the point explosion of Zeldovich [1] modified by Arnold et al [2]. It is interesting to note, that even if the expansion is not spherically symmetric due to high macroscopic forward velocity of the plume, the model of Zeldovich although not directly applicable is qualitatively correct. It is also worth noting that the Rankine-Hugoniot conditions for a plane shock wave may not be applicable here, as will be shown in the subsequent paragraphs.

3 DSMC simulation

Expansion of a plume of carbon atoms into an ambient atmosphere of nitrogen was simulated with the standard DSMC technique (Bird [3]). The pairs of molecules for collisions were selected according to the ”ballot box” algorithm of Yanitskiy [4]. The plume consisted of 10^{16} carbon atoms at initial temperature of 8000 K. Its initial shape was spherical, 3 mm radius, and it moved perpendicularly to the target with macroscopic velocity 20 km/sec. The ambient nitrogen gas had temperature of 300 K and pressures 10 Pa, 20 Pa and 40Pa (at this highest ambient pressure the plume radius was 1.5 mm). Dissociation of nitrogen molecules after collisions with fast moving atoms of the plume was taken into account. Here we present the results for ambient nitrogen pressure 20 Pa only.

4 Results

In Figure1 we show contour maps of the number density of carbon (left), the temperature (right) and the diagram of density and temperature distributions along the axis of symmetry of the plume (bottom), 247 nanoseconds after beginning of the simulation. In Figs. 2 and 3 we show similar diagrams for molecular and atomic nitrogen, respectively. In Fig. 1 the internal shock, directed towards the target, is clearly visible. As estimated from the earlier pictures (not shown here) its velocity is more than 3 times higher than the respective speed of sound. The corresponding density increase is much too low for such a shock speed, which indicates, that the shock is not fully developed. The temperature of carbon begins increasing above the initial level inside this internal shock however the main temperature increase takes place at larger distance from the target, in the ”contact layer”, where the highly energetic carbon atoms and ambient nitrogen molecules diffuse. In Figure2 the external shock in ambient nitrogen, directed from the target, can be seen. Similarly to the internal shock, this is not fully developed either. The density ratio across the shock moving in nitrogen at the speed of 20 km/sec would be close to 6, while here it is less than 2. The small decrease of density of nitrogen, visible in front of the external shock is due to dissociation; without taking dissociation into account this decrease is not present. Figure3 shows, that the atomic nitrogen is produced, as a result of dissociation, in the area where the energetic carbon atoms are scattered by ambient nitrogen molecules and attain high temperature at the cost of the former kinetic energy. When comparing all three figures shown above one can see that the temperatures of carbon and atomic nitrogen begin increasing farther ahead of the plume than that of molecular nitrogen. This may be because the majority of collisions of the carbon atoms (which in this area are very fast) with nitrogen molecules lead to dissociation. Hot atomic nitrogen is produced and the temperature of the remaining molecular nitrogen stays unchanged.

5 Conclusion

Expansion of a plume generated during laser ablation of materials was studied with the Direct Simulation Monte Carlo method. The plume consisting of carbon atoms expanded into atmosphere of molecular nitrogen. Dissociation of nitrogen molecules was taken into account. Two shocks were found: the external shock, moving forward in ambient gas in front of the plume, and the internal shock, moving backwards, inside the plume. This is in qualitative agreement with the model of spherical explosion, also predicting the existence of the same two shocks. However in the model of spherical explosion the internal shock could reflect from the centre of explosion and then move forward, while here if the plume moved with sufficient speed (which usually is the case) and vacuum was generated behind it, no reflection from the rear edge of the plume could occur.

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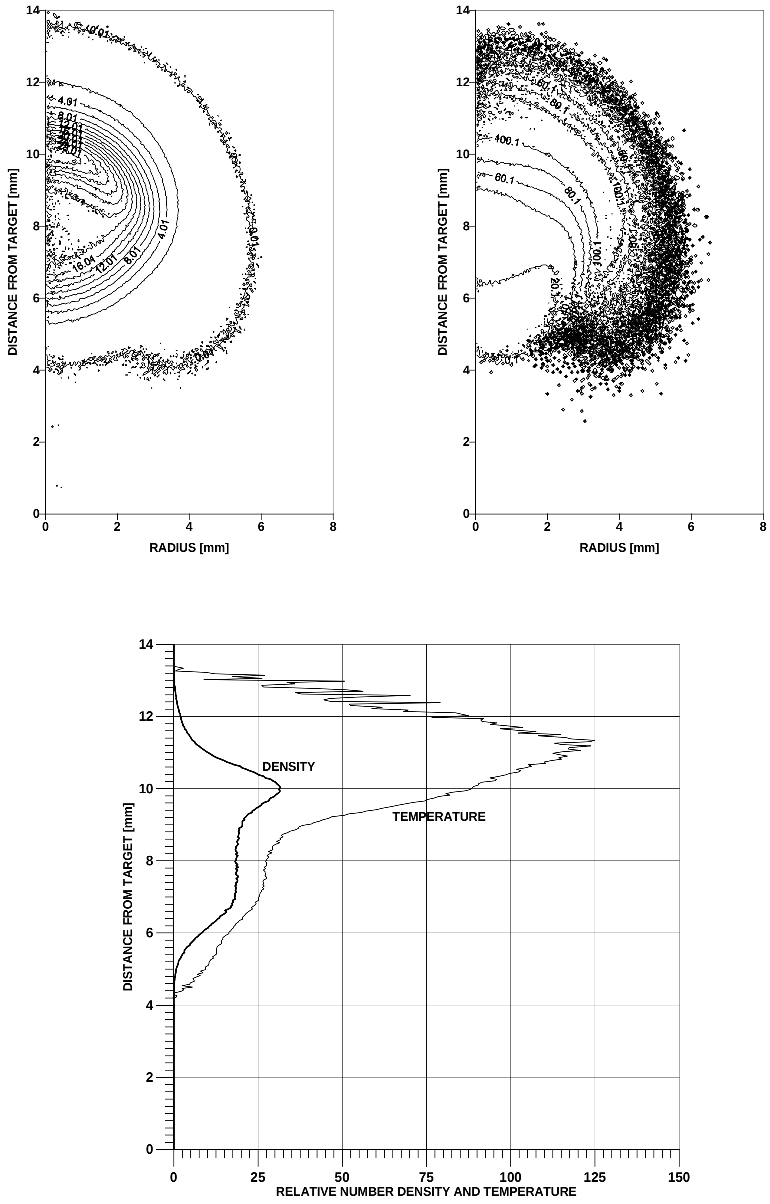

Fig. 1 Contour maps of relative number density of carbon (left), temperature (right), density and temperature distributions along axis of symmetry (bottom).
Reference number density: $0.473 * 10^{16} cm^{-3}$, reference temperature: 300 K.

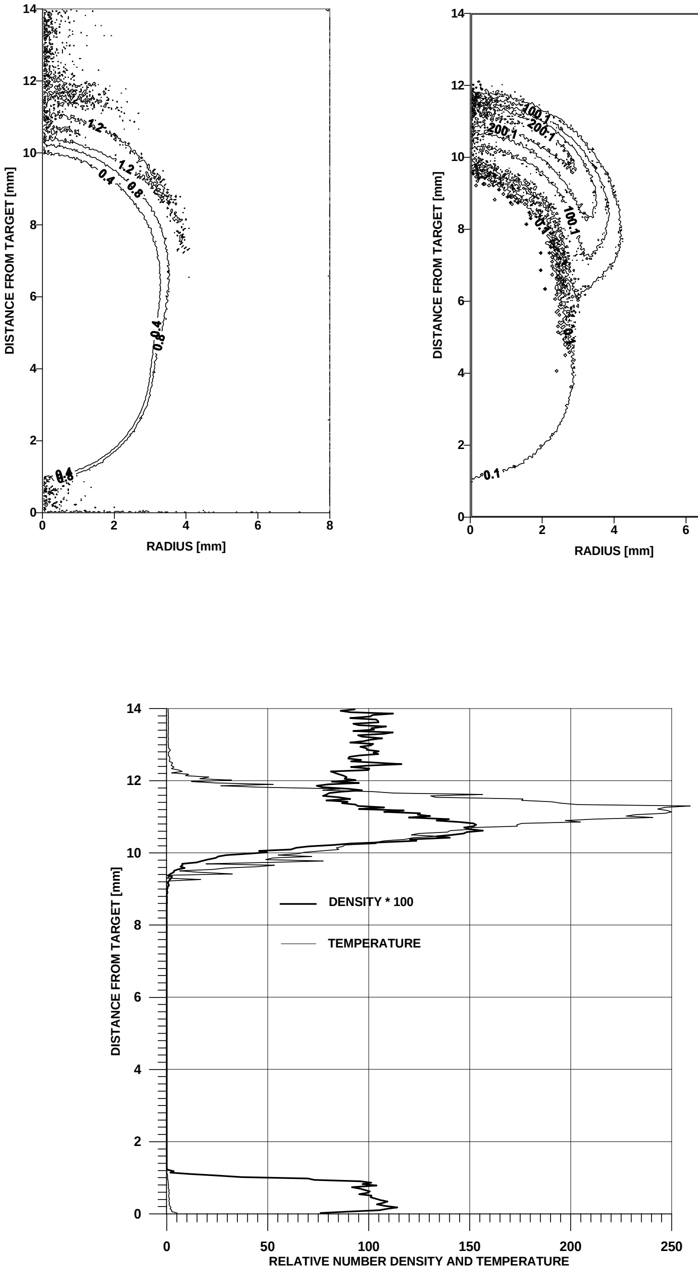

Fig. 2 The same as Figure1 for molecular nitrogen

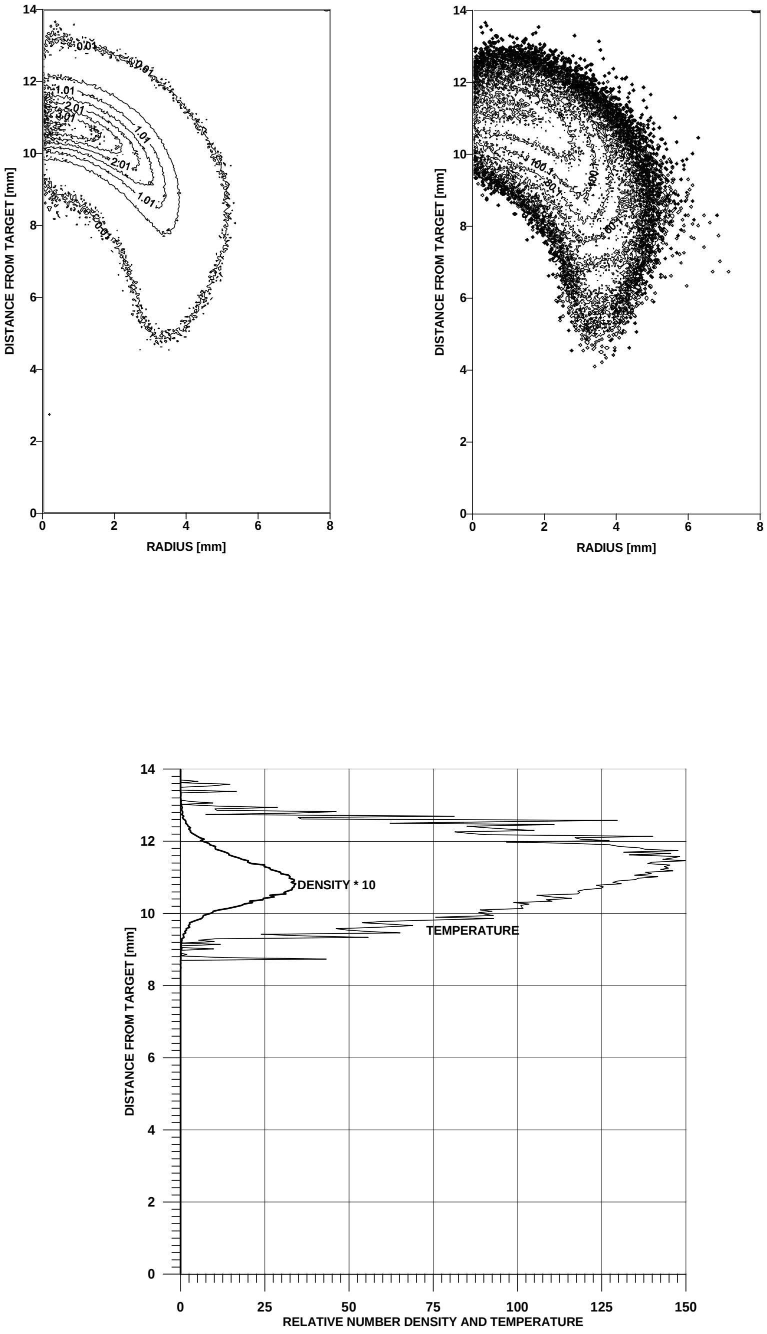

Fig. 3 The same as Figure1 for atomic nitrogen