LETTERS

Explosive boiling of metals upon irradiation by a nanosecond laser pulse

V.I. Mazhukin, A.A. Samokhin, M.M. Demin, A.V. Shapranov

Abstract. A repeated effect of explosive boiling has been found in metals exposed to a nanosecond laser pulse in the framework of molecular dynamic simulations combined with a continuum description of a conduction band electrons system. This effect can be used, in particular, as a marker of approaching critical parameters of the region in the irradiated matter.

Explosive (volume) boiling is inherent in the cases of quick, bulk energy release in a condensed medium, when the main role in the vapour phase formation is played by spontaneous homogeneous nucleation in a superheated metastable liquid [1]. Unlike absorbing dielectric fluids, the implementation of the explosive boiling of a metal under laser exposure is complicated by large values of the diffusivity and absorption coefficients, so that the question of experimental observation of this effect still remains virtually open, although its role in the near-critical behaviour of the nonequilibrium matter has been repeatedly observed (see, e.g., [2–5] and references therein). In this paper, using the numerical molecular dynamic simulations, the possibility of implementing the regime of repeated explosive boiling under nanosecond laser irradiation of metals, particularly of aluminium, is demonstrated.

Calculations were performed for a film containing 500 thousand atoms and having a thickness of 417 nm along the x axis, with free surfaces and periodic (period of 6.43 nm) boundary conditions along the z and y axes; the right side of the sample was irradiated. The computational domain in the x direction was 866 nm. The particles that reached the domain boundary were removed from the calculation. General method of calculation is similar to the well-known combined two-temperature model [5–7]; the details of the molecular dynamics calculations are also given in [8–10].

The calculations have been performed on a K-100 super-computer (Keldysh Institute of Applied Mathematics, RAS) using a self-developed parallel code for hybrid systems, including the processors and graphics accelerators. The code includes the widely used algorithms [11] of spatial decomposi-

tion of the domain and partitioning the domain into subdomains with the boundaries perpendicular to the longitudinal axis of the target, automatic balancing between these subdomains, and generation of a list of neighbours for a short-range EAM-potential [12]. The average calculation time of one variant using 12 graphic processors constituted 35 hours. In this case the absorption coefficient is $\alpha \sim 8 \times 10^5$ cm^{-1}, which, at the incident intensity $I > 1.5 \times 10^8$ W cm^{-2} and the absorbance of the irradiated surface $A = 0.22$, provided the rate of the energy input $\alpha AI > 10^{13}$ W cm^{-3}. The evaporation at lower intensities in the course of the entire simulation was of surface nature, just as it is described in [6, 7]. To shorten the calculation time, the initial equilibrium state of the film was chosen having a rather high temperature $T = 0.84T_{cr} \approx 6400$ K, which corresponds to the saturation pressure $P = 486$ bar. This model assumes the values of critical parameters to be as follows: $T_{cr} = 7600$ K, $P_{cr} = 1400$ bar, and $\rho_{cr} = 0.48$ g cm^{-3}.

At $I = 2 \times 10^8$ W cm^{-2} the first explosive boiling was observed at $t = 0.710$ ns after the heating began, and this process then repeated at $t = 1.17$ and 1.50 ns, while at $t = 1.80$ ns a 'doubled' explosion was observed, with almost simultaneous formation of two fragments. Before each boiling, a marked increase in the density fluctuations in the condensed phase near the irradiated surface was recorded, wherein the maximum temperature was fluctuating near 7000–7100 K, slightly increasing with time. Calculations of this variant continued until $t = 1.96$ ns. The difference between the electron (T_e) and ion (T_i) temperatures is negligible in this impact range, and is comparable with the magnitude of ion fluctuations in the framework of the molecular dynamics method.

Figure 1 shows the distribution of temperature and density of the film and its fragments at the various time moments (0.80, 1.40 and 1.92 ns), which corresponds to the first, second, and fourth-fifth boiling events, respectively. It is seen from the results of the calculations that the density of the separated fragment after some time passes through a maximum being notably higher than its initial value at the moment of separation, which coincides with the density on the right surface of the film. Such behaviour is due to the lowering of the fragment temperature, which is caused by the change in the relation between the energy absorbed by the fragment and the 'expenses' for evaporation. The density increase also contributes to the increase in pressure at the initial stage of explosive boiling. A further decrease in density is in turn associated with the discontinuities in the separated layer, mainly due to its general thinning, inasmuch the instabilities inherent to the evaporation process [13] are unable to manifest themselves during such a short time. We should emphasise that the fragment separation from the main mass of the material occurs due to the boiling effect and the formation of a cavity with a

V.I. Mazhukin, M.M. Demin, A.V. Shapranov M.V. Keldysh Institute of Applied Mathematics, Russian Academy of Sciences, Miusskaya pl. 4, 125047 Moscow, Russia; e-mail: shap@spnet.ru;
A.A. Samokhin A.M. Prokhorov General Physics Institute, Russian Academy of Sciences, ul. Vavilova 38, 119991 Moscow, Russia
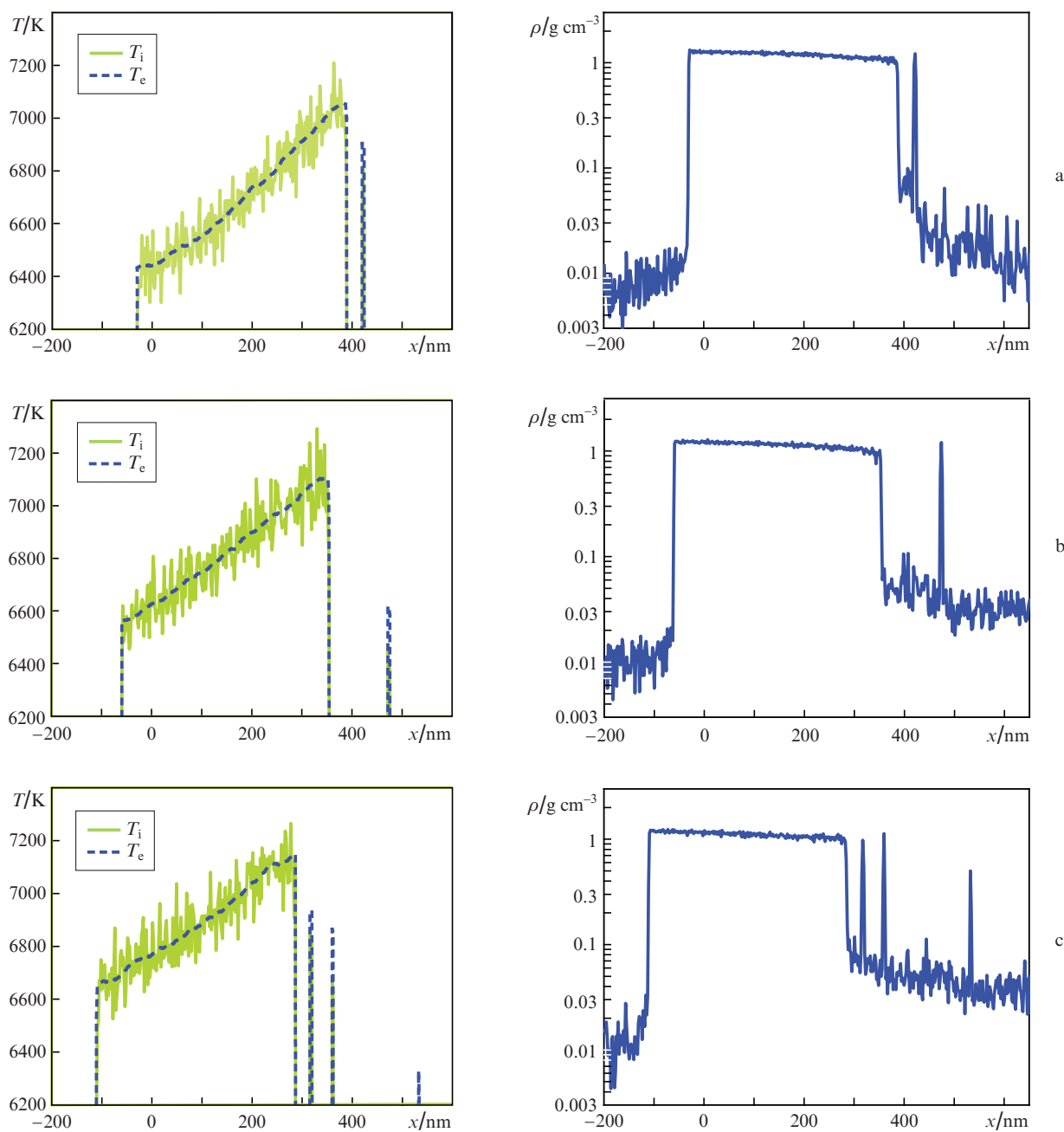
Figure 1. Distributions of temperature (left) and density (right) in the sample and calculation domain at the time moments (a) 0.80, (b) 1.40 and (c) 1.92 ns after the start of additional heating of the sample. The radiation is incident from the right.

higher pressure rather than due to inertia and the negative pressure which occurs in the unloading wave as a result of exposure to shorter laser pulses and has been a subject of active investigation in the recent years [5].

The temperature distribution across the film thickness approximately corresponds to the case of quasi-stationary evaporation, with taking into account the finiteness of the film thickness being comparable to the characteristic length of the temperature profile in the half-space, which is determined by the ratio χ/v, where χ is thermal conductivity and v is the motion velocity of the evaporation front along the film material [4]. The proximity to the stationary regime is consistent with the fact of substantial dependence of the first moment t_1 of boiling on the incident intensity – in the case of

$I = 1.75 \times 10^8$ W cm^{-2} the time t_1 increases up to 1.04 ns versus 0.71 ns at $I = 2 \times 10^8$ W cm^{-2}.

For large values of the dimensionless parameter ($\alpha\chi/v \gg 1$), the magnitude of the temperature maximum localised on the absorption length under the irradiated surface is small, which, together with the proximity of this peak to the surface, can significantly weaken the manifestation of the explosive boiling of metal under the action of laser radiation. Reduction of the temperature maximum is also due to reduction of the evaporation heat as it approaches the critical temperature T_{cr}, after passing of which the difference between the condensed and vapour phases disappears. In the supercritical ablation regime, the explosive boiling as the first-order phase transition is absent.

The numerical results obtained in the present work demonstrate, however, that this effect is sufficiently pronounced in the near-critical temperature region of the condensed phase even with no regard to the possible metal–insulator transition. Despite the relatively small thickness of the separated fragment (7 nm), the pressure jump of the explosive boiling of the metal exceeds by 30%–40% the previous back-blow pressure on account of the surface evaporation. In the case of the metal–insulator transition [2–4] accompanied by a decrease in the absorption coefficient α and the thermal conductivity χ, the excess of the maximum pressure of the explosive boiling over the previous level of the back-blow evaporative pressure may be greater. The use of the radiation with a smaller absorption coefficient may also contribute to the pressure increase.

Note that the almost two-fold pressure jump registered according to the change in the shock wave velocity over the irradiated target has been recently observed in the experiment [14] and attributed by the authors to the explosive boiling of the irradiated metal. It should be kept in mind, however, that the increase in pressure may also be caused by the appearance of the absorbing plasma layer. The microsecond pressure fluctuations associated with the occurrence of plasma above the irradiated surface have long been observed [15], but, so far as we know, nothing has been reported on the registration of the (sub) nanosecond pressure pulsations caused by the explosive boiling.

To clarify the role of different mechanisms in the formation of the back-blow pressure, further theoretical and experimental investigations on the peculiarities of the near-critical behaviour of metals under nanosecond laser exposure are required. Those investigations are aimed at gaining new information about critical parameters of metals to considerably complement not very definite data at hand [5]. The results of this work show that the manifestations of explosive boiling found during the numerical simulation can be used, for example, as experimental markers (when measuring the back-blow pressure) of approaching critical parameters under the conditions of nanosecond laser exposure of metals.

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