

## Thermal cycling of copper surface in pre-ablation regime under heating by ultraviolet nanosecond laser pulses

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The formation of surface relief on copper after exposure to nanosecond laser pulses at sub-threshold intensity in the condensed state has been experimentally studied. A system of micro-protrusions/depressions having a deformation character is formed in the irradiated zones near grain boundaries. Molecular dynamics simulation showed that the anisotropy of thermal expansion of differently oriented grains during cyclic heating to pre-melting temperature is the main reason for relief development, as thermal stresses arising in the subsurface layer exceed the yield strength of the material. Accumulation of defects with increasing energy density and number of pulses has been registered. The results are important for understanding the mechanisms of degradation of metal optics under thermocyclic pulsed loading.

**Keywords:** polished copper, nanosecond UV laser, optoplastic effect, grain boundaries, plastic deformation, molecular dynamics simulation.

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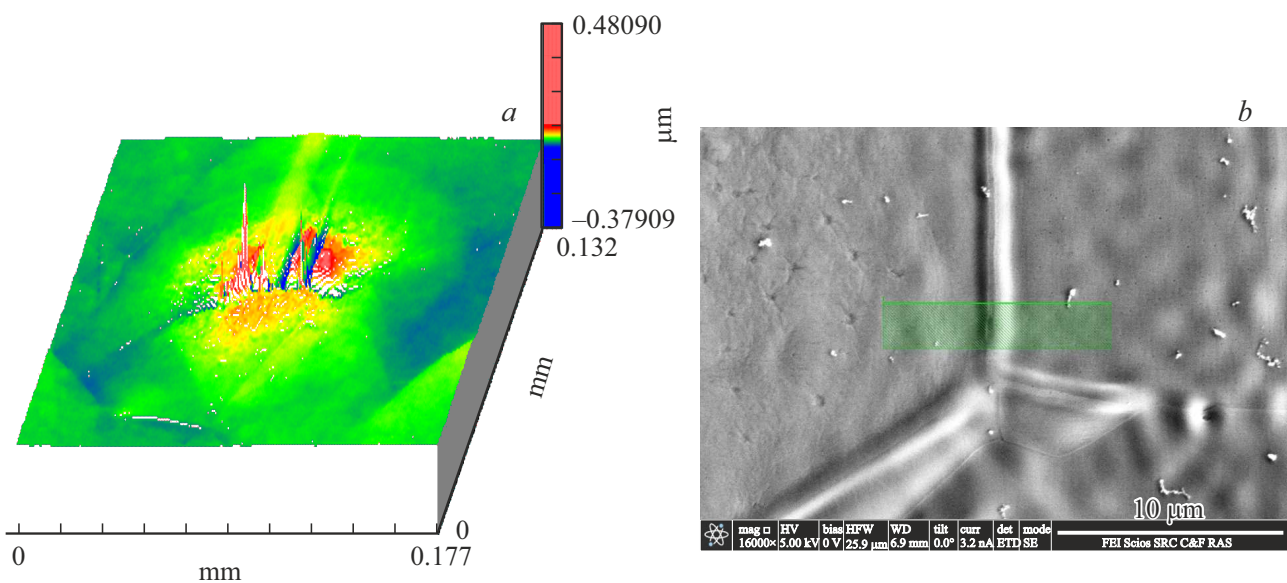
### 1. Introduction

The phenomenon of optical breakdown on the metal surface when exposed to laser radiation has long been studied [1–3]. Optical breakdown and the accompanying appearance of a laser crater on the surface of the material are usually considered as a classical threshold process. This approach is quite sufficient for the practical application of lasers in materials technology. Therefore, the processes preceding breakdown, occurring at pre-melting temperatures in the metal, have been studied noticeably less. We can only mention the theoretical studies of F. Mirzoev's work, for example, Ref. [4]. Unfortunately, purposeful experimental work in this area is not yet available. Sometimes there were scattered works that did not find a theoretical explanation, for example [5–8].

A series of experimental studies of the optical resistance of copper mirrors to the radiation of a pulsed CO<sub>2</sub> laser (pulse duration 1.7 ns) in vacuum was performed in Refs. [9,10]. On their surface, traces of damage

were found, later called laser-induced periodic surface structures (LIPSS). A theoretical analysis of these results was carried out in Ref. [11]. According to V.S. Makin, the surface electromagnetic wave energy was excited and dissipated by incident radiation in the vacuum system—plasma layer—metal. Interest in fatigue processes in metal optics has intensified due to the problems of using mirrors made of stainless steel in ITER [12].

However, in recent years, a series of papers has been published [13–16], where the results of laser exposure to metals occurring at pre-melting temperatures and preceding breakdown, that is, at maximum permissible radiation loads, have been experimentally investigated. The mechanisms of degradation of the polished surface of copper samples with a thickness of 10 mm when exposed to frequency-pulse laser radiation (wavelength  $\lambda = 355$  nm, duration  $\tau = 10$  ns, repetition rate 10 Hz) in the preablation mode were studied. It has been established that when exposed to radiation (energy density of the order  $W_p = 0.1–1.0$  J/cm<sup>2</sup>), an irreversible microburst occurs on the polished surface of



**Figure 1.** (a) 3D profilogram of a laser spot after exposure to 15 UV laser pulses; (b) SEM image with a rectangle indicating the lamella cut-out area.

copper and a number of its alloys in the area of the laser spot. This happens without changing the phase composition of the material, in a condensed state. The phenomenon is called the optical plastic effect. In this paper, an in-depth experimental and theoretical study of this process on polished samples of oxygen-free copper using methods of modern materials science is carried out.

## 2. Experimental methodology

Using a combination of optical profilometry, confocal scanning laser and scanning electron microscopy (SEM), as well as transmission electron microscopy, the nature of the created structure was revealed. The initial examination of the surface of the material was performed on a Zygo NewView 7300 optical profilometer. Further study of the microstructure of the near-surface layer was performed in thin foils (lamellae) using a Tecnai Osiris transmission electron microscope (TEM) (accelerating voltage 200 kV). The lamellae, approximately  $8 \times 7 \mu\text{m}$  in size, were cut perpendicular to the sample surface by ion thinning with a focused beam. The process was carried out in the column of the FEI Scios scanning electron-ion microscope (CUC of FSRC „Crystallography and Photonics“). The method of manufacturing lamellae is described in detail in Ref. [17].

## 3. Experimental results and discussion

Figure 1, *a* shows a 3D profilogram of a laser spot that appeared on the copper surface (size  $180 \mu\text{m}$ ) after exposure to planar polarized radiation from 15 laser pulses (wavelength 355 nm, duration 10 ns, repetition rate 10 Hz,

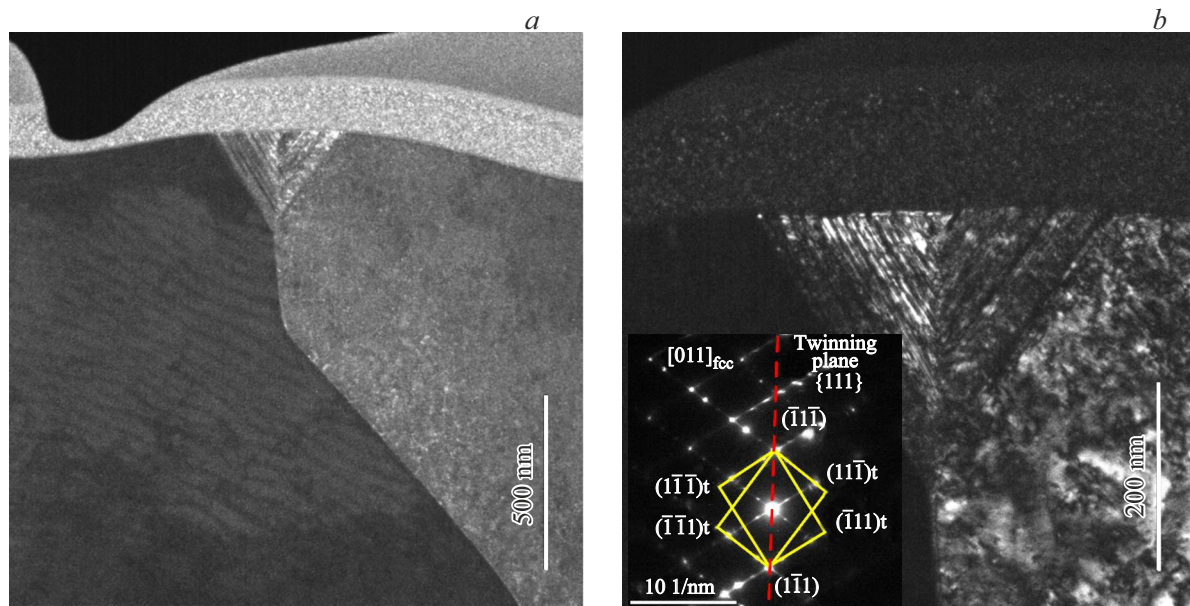
pulse energy density  $0.6 \text{ J/cm}^2$ ; laser parameters and exposure technique corresponded to the work [13–16]).

Figure 1, *b* shows the place where the lamellae are cut out of the test sample. A detailed analysis of the microstructure of the lamellae obtained using transmission electron microscopy (see Figure 2) showed that a characteristic system of protrusions and depressions is formed in local areas near the grain boundaries. The height difference reaches up to 500 nm. At the same time, in a thin near-surface layer ( $\sim 2 \mu\text{m}$ ), heated during the pulse to pre-melting temperature, traces of irreversible plastic deformation were found near the grain boundaries. These are nanoscale twin formations, dislocations, and small-angle dislocation boundaries. During the time between pulses, the surface cools completely and irreversible changes are fixed. With an increase in the number of pulses, as well as the density of their energy, the accumulation of defects is recorded.

The configuration of the resulting defective structures shown in Figure 2 demonstrates the active role of the dislocation mechanism in the relaxation of residual internal stresses occurring on the copper surface during pulsed laser thermal cycling in the additional melting mode.

The deformations and stresses in a cubic single crystal were calculated using the example of copper during its nanosecond heating at 1000 K using the linear theory of elasticity. It is shown that for all crystal orientations, the stresses that arise exceed the static yield strength of copper, which does not exceed  $Y \approx 0.5 \text{ GPa}$ , that is, plastic deformations must inevitably occur under the experimental conditions discussed above.

Moreover, within the framework of the linear theory of elasticity, the analysis is also applicable for smaller temperature differences. Since the range of calculated stresses is approximately 4 times higher than the yield strength, plastic



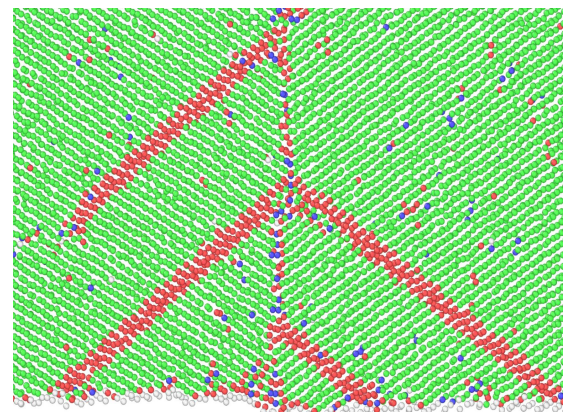
**Figure 2.** Microstructure of the sample in the area with a protrusion: *a* — light field; *b* — twin structure near the protrusion. The orientation of the grains in the axis of the  $[011]$  FCC zone and the microdiffraction pattern in this area of the sample. The microdiffraction pattern includes both the matrix grain and the twin plates, which are several nanometers thick.

deformations should be expected already when heated at 250 K. However, when copper is rapidly heated by a laser pulse with a duration of 1–10 ns, the experimental strain rate is estimated as  $\sim 10^6$ – $10^7$  s $^{-1}$ . In this case, the dynamic yield strength, at rates exceeding  $10^5$  s $^{-1}$ , becomes significantly higher than the static value [18,19].

#### 4. Molecular dynamic modeling

To illustrate the plastic deformation of polycrystals during thermal cycling, molecular dynamic (MD) modeling of copper samples with sharply different sizes was performed: a model copper bicrystal with grain orientation corresponding to the experimental data shown in Figure 2, and a polycrystal with random grain misorientation. The method made it possible to evaluate the atomic features of deformation of various copper grains during rapid heating/cooling and high deformation rates, which is extremely difficult to do analytically.

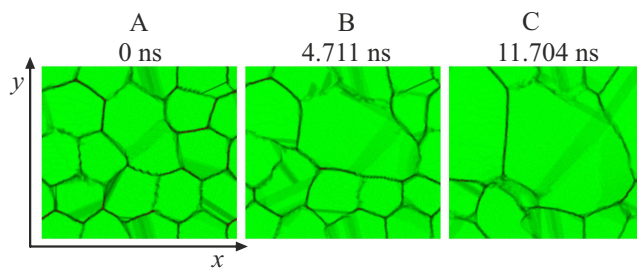
For the first MD simulation, a unit cell of a copper crystal with a size of  $64 \times 6.6 \times 26$  nm was used. The axis  $z$  is oriented along the direction  $\langle 111 \rangle$ , the axis  $y$  is oriented along the direction  $\langle 211 \rangle$  and the axis  $x$  is oriented along the direction  $\langle 011 \rangle$ . The centers of the formed grains are located at points  $0.5 \times 0.5 \times 0.25$  and  $0.5 \times 0.5 \times 0.75$  (in units of sample size). Molecular dynamic modeling using the lammps program [20] included relaxation of atoms to a minimum of energy, annealing at 300 K, and simulation of heating-cooling cycles simulating the effect of a laser pulse (1200 K, 1.4 ns), which led to the formation of deformation twins and the height difference of the surface is 1 nm



**Figure 3.** A cutout of the near-surface layer of a model copper sample consisting of two grains. The green color indicates atoms with a local environment as in the FCC structure, red — HCP structure (which corresponds to atoms belonging to deformation twins), white — atoms on the surface of the sample. The structure was analyzed in the OVITO program [21]

(Figure 3). Additional thermal cycling cycles (300–1200 K) did not enhance the relief due to the small crystallite sizes and limited simulation time, which is incomparable with real experiments where diffusion relieves stress over longer periods.

Then a large-scale MD simulation was carried out (on a much larger scale). Enlarged sample of 16 grains longitudinal along the axis  $z$  with a hexagonal cellular structure and dimensions  $L_z = 100.1$  nm along the axis  $z$ ,  $L_y = 40.7$  nm along the axis  $y$  and  $L_x = 46$  nm along



**Figure 4.** A change in the initial pencil configuration of copper grains as a result of exposure to 5 cycles of laser pulse heating to a temperature of  $T \approx 1300$  K for about 1.2 ns and subsequent natural cooling to room temperature. A — at the beginning, B — after 3 cycle, C — after 5 cycle.

the axis  $x$ , contained up to  $2 \cdot 10^7$  atoms. The boundary conditions along the axis  $x$  and  $y$  were periodic, the boundary conditions along the axis  $z$  were free. Initially, one grain contained about 1 million atoms. The orientation of the crystal grains was arbitrary, as were the mutual orientations of neighboring grains. In order to better agree with the experimental melting point and surface tension (energy), an updated version of the Zhakhovsky potential was developed [22].

5 pulses were simulated, that is, the sample underwent a cycle of homogeneous heating 5 times to a pre-melting temperature  $T \approx 1300$  K for a time of approximately 1.2 ns, followed by cooling to room temperature (Figure 4).

The performed molecular dynamic modeling has shown that the main factor in the appearance and development of a microburst on the surface of a copper sample is the anisotropy of thermal expansion of variously oriented metal grains (crystallites) during cyclic heating to pre-melting temperatures and subsequent cooling to the initial state. Theoretical analysis has shown that the thermomechanical stresses occurring in the heated layer exceed the yield strength of the material.

## 5. Conclusion

Cyclic pulsed thermomechanical loads are often found in various fields of industry. Understanding the specifics of these processes is extremely important, both for fundamental science and for practical use. The results obtained have clarified the processes occurring in the metal near the melting point. They will allow us to deepen the fundamental understanding of the physical features of metal structure degradation during fatigue processes that occur under extreme thermocyclic loads. In particular, these results can be used in the development of methods for improving the operational resistance of metal optics.

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## Conflict of interest

The authors declare no conflict of interest.

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