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Ablation of a nanostructured metal surface by ultrashort X-ray pulses

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ABSTRACT

Using molecular-dynamics simulation, we study the interaction of an ultrashort X-ray pulse with an Al surface. The surface has a periodic grating structure consisting of alternating ridges of height 80 nm and width 80 nm, separated by trenches of width 160 nm. After irradiation with an ultrashort (0.2 ps) X-ray pulse with a fluence above the ablation threshold we observe that the ridges first disintegrate into a foamy mixture of melt and gas bubbles, which grow faster than those in the trenches. Due to the interference of tensile pressure build-up below the ridges and the trenches, the material does not spall. At the concave edges, jets are emitted with velocities of around 1000 m/s, which may ultimately lead to the creation of finer surface structures.

Laser irradiation of a surface leads to the ablation of the material if the laser intensity is sufficiently high. For metallic targets the processes leading to ablation by ultrashort pulses have been studied intensely [1–4]. At and slightly above the ablation threshold, mechanical spallation is responsible for ablation. The high compressive pressure induced by the irradiation is reverted by reflection at the surface to a tensile pressure; if this tensile pressure surpasses the tensile strength of the material, it may tear. This process usually occurs in the molten phase.

Since ablation is a mechanical process it may be influenced by the geometry of the irradiated target. The length scale of the pressure profile is governed by the laser absorption depth; surface structure sizes of this scale may hence have a profound influence on the shape and propagation of both the compressive and tensile pressure pulse and hence the ablation. While visible light is attenuated on a scale of 10 nm, only tiny nanostructures will influence the ablation process. For X-ray irradiation with attenuation lengths in the order of 100 nm, influences can be expected for surface features of a size relevant for experiments. Recent machines like FLASH, Hamburg, or the Linear Coherent Light Source (LCLS), Stanford, supply powerful and ultrafast XUV and even X-ray pulses.

In this paper we analyze the processes leading to ablation in a periodically nano-structured Al target irradiated by an ultra-short X-ray pulse. The structure length and laser attenuation length are of the order of 100 nm. We shall demonstrate that the structured surface leads to ablation patterns that are strongly different from those of a planar surface.

The target consists of an Al crystal which is 240 nm wide. On its surface, a 80-nm wide ridge with height of 80 nm alternates with a 160 nm wide trench. The film is 121 (41) nm thick below the trench (ridge). Periodic boundary conditions extend this ridge/trench structure to a periodic grating, see Fig. 1. In the third dimension, the target is 6.4 nm thick; here again periodic boundary conditions are applied. The number of atoms in the target is 6.5×10^6.

The laser has a Gaussian time distribution, $f(t) = (1/\sqrt{2\pi\sigma^2})\exp(-0.5(t-t_0)^2/\sigma^2)$, with $\sigma = 0.2$ ps and $t_0 = 1$ ps. The energy absorbed per atom at the target surface – and integrated over the laser pulse duration – amounts to $E_0 = 1.21$ eV. The depth dependence will be discussed below, Eq. (2).

The energy absorbed per atom $E_0 = 1.21$ eV is above the ablation threshold for a planar Al target, 1.0 eV/atom [5]. We treat here the case of an X-ray laser with a long attenuation length, $\lambda = 100$ nm [6]. This avoids issues concerning near-field phenomena, i.e., surface

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