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Melting of Al Induced by Laser Excitation of 2p Holes

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Novel photon sources—such as XUV- or X-ray lasers—allow to selectively excite core excitations in materials. We study the response of a simple metal, Al, to the excitation of 2p holes using molecular dynamics simulations. During the lifetime of the holes, the interatomic interactions in the slab are changed; we calculate these using WIEN2k. We find that the melting dynamics after core-hole excitation is dominated by classical electron–phonon dynamics. The effects of the changed potential surface for excited Al atoms occur on the time scale of 100 fs, corresponding to the Debye time of the lattice.

Keywords: Laser Materials Processing, XUV Irradiation, Molecular Dynamics, Al

Ultrafast laser-induced melting of metals has been studied theoretically in the past by computer simulation and many aspects are by now well understood.[1–6] Such studies consider the action of a visible-light (VIS) or ultraviolet (UV) laser, which conveys the photon energy to the conduction electrons of the metal. Electron–phonon coupling then equilibrates the energy with the lattice, which is heated and melts. Aspects such as the superheating of the lattice, the nucleation of the liquid phase, or the influence of pre-existing lattice defects, for example, grain boundaries, have been studied.

Apart from this ‘conventional’ energy transfer via the conduction electron gas, another route of heating the lattice was detected in several materials; the accompanying melting process was termed *non-thermal melting*, as lattice disordering and melting occur so quickly—on the timescale of several 100 fs—that the lattice is not in (local) thermodynamic equilibrium. The process operates via the changed interactions that lattice atoms experience as a consequence of the laser-excited electrons. It has first been found in covalently bonded materials

crystallizing in the diamond structure such as C or Si [7–10] and, more recently, also in a wider class of semiconducting and semimetallic materials, for example, in InP [11] and Bi.[12] On the microscopic scale, non-thermal melting can be distinguished from conventional melting by fractionally diffusive atomic pathways.[13]

In the present paper, we inquire how laser-induced changes of the interatomic interaction potential of a simple metal, Al, influence the melting process. VIS or UV lasers will not be able to induce such changes.[14] However, extreme ultraviolet (XUV) pulses with an energy of 75 eV are able to selectively excite 2p core holes in Al atoms. We study their effect on the subsequent lattice dynamics.

We assume the laser pulse to have a Gaussian time distribution with maximum at time $t_0 = 0$ and width σ ,

$$S(t) = \frac{E_0}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\left(\frac{t-t_0}{\sigma}\right)^2\right]. \quad (1)$$

Here E_0 is the total energy absorbed by the electrons per unit volume. Due to the large penetration depth of 75 eV

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