CFEL SCIENCE

SEMINAR

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CFEL-bldg. 99, seminar room IV

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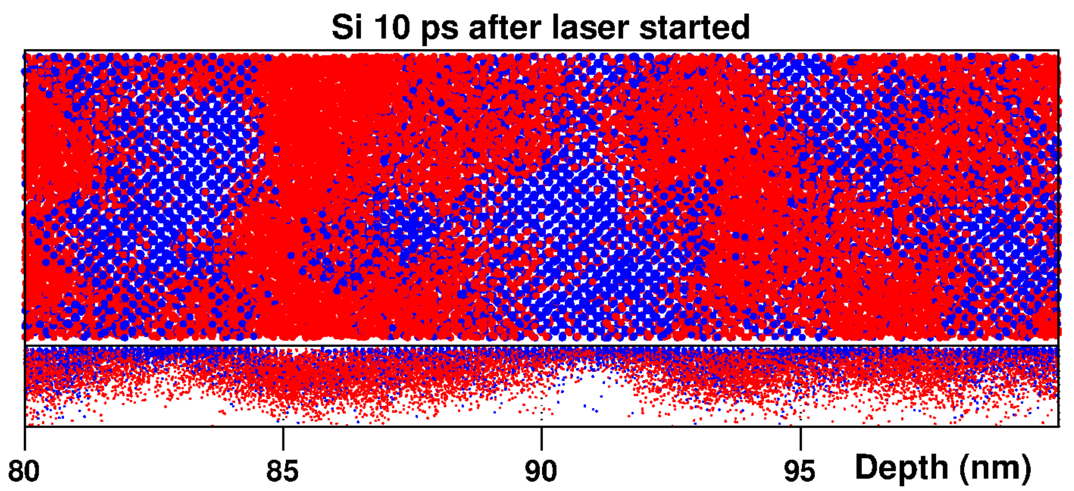
Atomistic-continuum modeling of ultrafast laser-induced melting of silicon targets

In this work, we present simulations of ultrafast laser-induced melting of silicon using a combined atomistic-continuum model. The laser light absorption, strong generated electron-phonon nonequilibrium, fast heat conduction, and diffusion of photo-excited free carriers are described with a continuum TTM-like model (called nTTM), whereas the kinetics of transient non-equilibrium phase transitions is addressed with classical molecular dynamics (MD) method on the atomic level. Such combined MD-nTTM model allowed to investigate the effect of laser-induced pressure and temperature of the lattice on the ultrafast melting kinetics. Two competing melting mechanisms, heterogeneous and homogeneous, were identified in our big-scale simulations. Apart from the classical heterogeneous melting mechanism, the nucleation of the liquid phase homogeneously inside the material significantly contributes to the melting process.

It is well-known that the interatomic interactions in semiconductors may be strongly influenced by hot laser-excited carriers. To account for such non-thermal effects, we further performed preliminary MD simulations with a new interatomic potential, designed to reproduce ab initio calculations at the laser-induced electronic temperature of 18946 K. The simulations demonstrated that, similarly to thermal melting, nonthermal phase transition occurs through nucleation. A series of simulations showed that higher (lower) initial pressure reinforces (hinders) the creation and the growth of nonthermal liquid nuclei.



Host: Robin Santra – CFEL-DESY Theory Division