Atomistic-Continuum Modeling of Laser-Induced Phase Transitions in Silicon: Melting, Ablation, Solidification, and Amorphization

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Modern semiconductor applications demand precise laser processing at the nanometer scale, requiring a detailed understanding of phase transition and structural modification mechanisms. Accurate control over laser-induced processes in semiconductors is essential for generating predesigned surface structures and modifying the surface properties. In this study, we present a numerical investigation of non-equilibrium laser-induced phase transitions in silicon (Si) using a hybrid atomistic-continuum model [1]. The model combines the strengths of Molecular Dynamics (MD) simulations for atomistic-scale descriptions of non-equilibrium phase transitions with a continuum approach to account for the effect of laser-generated free carriers. As compared to the ordinary continuum or MD approaches, this advanced framework, therefore, captures the kinetics of melting and ablation phenomena on one hand, and generation and diffusion of the electron-hole pairs, thermal diffusion, and the electron-phonon coupling processes during laser energy deposition on the other hand, Fig. 1. We applied the model to determine the melting depth as a function of fluence for a 100 fs laser pulse at 800 nm. The results show that the stand-alone continuum approach underestimates the melting threshold as compared to the hybrid atomistic-continuum model by 46% originating from the detailed description of the melting kinetics. Additionally, we explored the effect of crystal orientation on melting dynamics and compared the results with the corresponding experimental measurement. Finally, the MD model is used to identify the conditions leading to the amorphization of the Si surface and corresponding cooling rates are referred to the experimental conditions. These findings provide valuable insights into experimental observations of Si surface structuring induced by ultrashort laser pulses.

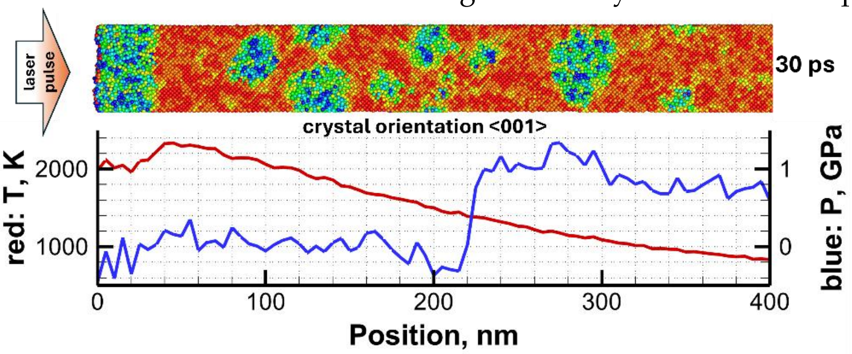

Figure 1: The atomic configuration of part of the Si target, irradiated by 100 laser pulse at the incident fluence of 0.32 J/cm^2, at 30ps after the pulse. The atoms are colored by Central Symmetry parameter (CSP) for distinguishing between solid (CSP > 0.97) and liquid (CSP < 0.97). Below, the profile of temperature and pressure are shown for the same spatial scale and at the same time.

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References:

[1] V.P. Lipp, B. Rethfeld, M.E. Garcia, and D.S. Ivanov, "Atomistic-Continuum Modeling of Short Laser Pulse Melting of Si Targets", *Phys Rev B* **90**, 245306 (2014).