Atomistic simulation of silicon film ablation by ultrashort laser pulse

Gordeev I S[1,2,@] **and Starikov S V**[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] ilya.gordeyev@phystech.edu

Femtosecond laser ablation removal of condensed matter is one of the key processes in nano- and microscale surface treatment of materials. The laser printing method makes it possible to cheaply and massively create nanostructures with a silicon base. However, despite the promise of this technology, the fundamental processes underlying femtosecond laser ablation are still poorly understood. In practice, this can manifest itself in the form of random deformations of the surfaces of ablation spots. However, ablation mechanism for silicon is not fully understood. In this paper, molecular dynamics coupled with a two-temperature model is used to study the interaction of a femtosecond laser pulse with silicon. The obtained simulation results for bulk silicon ablation are in good agreement with experimental data. The key role in this process is played by a significant change in density during melting of the semiconductor. The constructed model makes it possible to predict the behavior of silicon films irradiated with a femtosecond laser pulse. The study of threshold energy inputs and pressure profiles during ablation for thin films was carried out in 2D and 3D cases.