Novel excitation-induced non-thermal effects and ablation mechanisms in silicon from atomistic simulations with a thermal spike model

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The purpose of this work is to model laser ablation of silicon on an atomistic scale in combination with a mesoscale model for the description of the electron-phonon interaction and an electron-temperature dependent interaction potential.
The well-known continuum two-temperature model (TTM) for solids with highly excited electrons is extended from metals to silicon by explicitly taking charge carrier transport effects into account. The model is combined with classical molecular dynamics (MD) simulations to study laser ablation in silicon where the charge carriers are created by the absorption of laser light. The simulation model is further enhanced by extending the modified Tersoff potential (MOD) to a dynamical carrier excitation-dependent Tersoff Potential (MOD*) [1,2] that reproduces the change of bond strength following the excitation [3,4].

As an application we investigate the non-thermal material dynamics of strongly excited silicon during ultra-fast laser ablation. In contrast to metals, silicon shows significant excitation-dependent interatomic bonding strengths, which gives rise to a number of unique material dynamics like non-thermal melting, Coulomb explosions and altered carrier heat conduction due to charge carrier confinement. In this study, we report novel non-thermal ablation mechanisms in the ultra-fast single shot laser ablation of silicon and perform large scale massive multi-parallel simulations on experimentally achievable length scales with atomistic resolution [5].

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References:

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