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Ab initio simulations of ultrafast laser-induced structural instabilities in transition metals

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Structural modification and phase transition in materials subject to intense laser excitation is an area of intensive research. Occurring dominantly via electronic excitation, ultrafast laser processes are impacted by the influence of hot electrons on the lattice dynamics. We discuss the possibility to trigger atomic disordering for transition metals under non-equilibrium electron-phonon conditions, for Cr, Ni, and Ti. These transition metals have different degree of d-band filling and crystalline arrangements. Using first-principles calculations (DFT) we illustrate the charge distortion in the cold crystalline arrangement due to electronic heating, along with an entropy increase. In particular, electronic free energy calculations reveals a possible solid destabilization for an electronic temperature around 2 eV. A raise of electronic pressure and entropic blast forces drive this destabilization mechanism. Simulating uniaxial cell expansion, pressure relaxation indicates a loss of lattice stability on particular orientations, as indicated in phonon spectra showing imaginary frequencies, affecting the lattice cohesion in an anisotropic way. We try to correlate phonon instabilities under electronic temperature and uniaxial strain with electronic density redistribution along the relaxation direction.

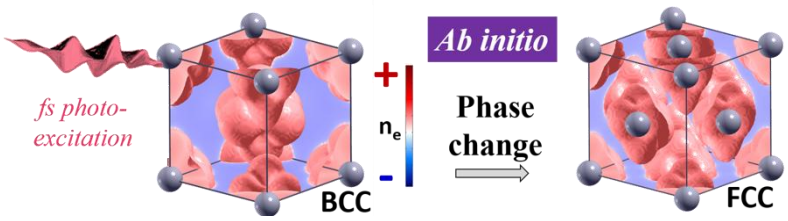

Figure 1 : Example of crystal transformation induced in a body centered cubic metallic lattice (Tungstene) due to a reorganisation of the nonequilibrium electronic structure.