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Ab initio simulation of intense short-pulse laser irradiation of metals and semi-conductors VANINA RECOULES, CEA/DIF - Departement de Physique Theorique et Appliquee, PIERRE-MATHIEU ANGLADE, CECAM, JEAN CLÉROUIN, CEA/DIF, GILLES ZÉRAH, CEA/DIF, STEPHANE MAZEVET, Los Alamos National Laboratory — The effect of intense ultra-laser irradiation on crystal stability is not completely elucidated. Ultrashort laser pulses heat electrons to a very high temperature and leave the lattice relatively cool since the heat capacity of electrons is much smaller than that of lattice. This non-equilibrium system can be described as two subequilibrium systems : the hot electrons and a cold lattice. We studied the effect of this intense electronic excitations on the interatomic forces and the possible melting of the underlying lattice for a semi-conductor (Si) and two metals (Al and Au). We used *ab initio* linear response to compute the phonon spectrum in the Density Functional Theory framework for several electronic temperatures ranging from 1 to 6 eV. We found that semi-conductors and metals behave in an opposite ways when increasing electronic temperature. Phonon instability appears in silicon at a electronic temperature of 1.5 eV inducing the melting of the lattice. Gold samples become more stable. The Debye temperature was deduced from the phonon spectrum and using the Linderman criterion, we showed that gold undergoes a sharp increase of its melting temperature under intense laser irradiation. The same effect is observed for aluminium.

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