THE ELECTRONIC STRUCTURE, LATTICE DYNAMICS, AND ELECTRON-PHONON COUPLING FACTOR OF METALS UNDER NON-EQUILIBRIUM HEATING

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We present results of ab initio calculations taken to study the electronic structure, phonon spectrum, and electron-phonon coupling factor $G(T_e)$ of several metals (Ag, Au, Pd, Pt, Rh, Ir, W, and Ta) at different electron temperatures T_e (~10^4 K) and the "cold" crystal lattice. We studied the effect of changes in the electronic structure under electron heating on lattice dynamics and the electron-phonon coupling factor. The outcomes of our study suggest that the evolution of lattice dynamics is quite well correlated with changes in the electronic population of the outer *d*-bands with the growing T_e. The decrease of *d*-electrons results in crystal hardening because the Coulomb potential screening of nuclei reduces, while their increase leads to the growth of the electronic screening and lattice softening. Our calculations show that in the initial phase of heating (T_e < 20 kK), the growth of the electron temperature in fcc metals may result in both lattice hardening (Pd, Pt) and lattice softening (Rh, Ir), or quite weak changes in lattice dynamics (Ag, Au). However, lattice softening never makes fcc metals lose their dynamic stability. At higher temperatures (T_e > 20 kK), the tendency to lattice hardening always prevails in them. As for the bcc metals, they are found to lose their dynamic stability as the electron temperature increases above 20 kK. Performed investigations show that the indicated tendency to change lattice dynamics is global among metals. It is also shown in this paper that differences in the electronic structures of metals strongly influence the behavior of the electron-phonon coupling factor as dependent on the electron temperature.