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Electron-Phonon Interaction and High-Temperature Thermodynamics in Vanadium Alloys and Compounds OLIVIER DELAIRE, MAX KRESCH, MATTHEW LUCAS, JORGE MUNOZ, CALTECH, JIAO LIN, BRENT FULTZ, CALTECH, CALTECH TEAM — Inelastic neutron scattering was used to measure the phonon densities of states (DOS) for pure V and V-6%X solid solutions, and for the A15 compounds V3Si, V3Ge and V3Co, at temperatures from 10 K to 1300 K. Pure V and the A15 superconductors V3Si and V3Ge exhibit an anomalous anharmonic stiffening of phonons with increasing temperature up to 1000 K. In V, this anharmonicity is suppressed by Co and Pt, but not by iso-electronic Nb solutes. Non-superconducting V3Co exhibits a normal quasi-harmonic softening. The electronic density of states was calculated from first-principles DFT methods for all alloys and compounds. The materials whose phonons behave anomalously also exhibit sharp peaks below the Fermi energy in their electronic DOS. The phonon-enhanced thermal smearing of these sharp features results in reduced screening of nuclear motions and stiffer phonons. These results show that the EPI can influence the phonon thermodynamics at temperatures up to 1000 K.

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