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Electron-Phonon Interaction and High Temperature Thermodynamics of Vanadium Alloys and Compounds

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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 10K to 1300K. Pure V and the A15 superconductors V3Si and V3Ge exhibit an anomalous anharmonic stiffening of phonons with increasing temperature up to 1000K. 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 electron-phonon interaction can influence the phonon thermodynamics at temperatures up to 1000K.

Mardi 18 Décembre 2007 à 15h

N.B : ***Les visiteurs de nationalité étrangère hors Union Européenne sont priés de bien vouloir avertir impérativement 3 semaines à l'avance - les visiteurs de l'Union Européenne 1 ou 2 jours avant le séminaire - le Secrétariat du Service de leur entrée sur le Centre :***

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