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Heat capacity anharmonicity in elemental vanadium and V₉₃Co₇

JORGE MUNOZ, The University of Texas at El Paso, OLIVIER DELAIRE, BRENT FULTZ, California Institute of Technology — The specific heats of elemental vanadium and V₉₃Co₇ with body-centered cubic crystal structure were measured by differential scanning calorimetry from room-temperature to 1400C. The results were compared to the harmonic phonon contribution, the electronic contribution, and the expansion against the bulk modulus contribution to the total heat capacity. The harmonic phonon contribution was obtained from the phonon densities-of-states, measured using inelastic neutron scattering. The electronic contribution to the heat capacity was obtained from ab-initio electronic band structure calculations. For the thermal expansion contribution, the room-temperature bulk and shear moduli were calculated after sound velocity measurements done by ultrasonic transduction; the coefficients of thermal expansion were measured from room-temperature up to 700C using thermomechanical analysis. The study shows that the source of the heat capacity anharmonicity in the measured samples is phonon-phonon interaction.

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