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Electronic structure and high-temperature lattice dynamics of B2-ordered FeTi JORGE MUNOZ, LISA MAUGER, California Institute of Technology, MATTHEW LUCAS, Air Force Research Laboratory, BRENT FULTZ, California Institute of Technology — FeTi is a brittle, non-magnetic B2-ordered (CsCl-type) intermetallic alloy with an electronic structure similar to that of Cr. The Fermi level lays in a deep pseudo-gap and therefore, the bonding and anti-bonding orbitals are well separated. Inelastic neutron and x-ray scattering were used to measure the phonon spectra at temperatures up to 1035 K. Complementary measurements up to pressures of 47 GPa were used to obtain quasi-harmonic Grüneisen parameters. Ab-initio calculations of the force constants and Born-von Kármán fits to the data show that the bonds between second nearest neighbors are much stiffer than that those between first nearest neighbors, but the rate of softening with temperature is higher for the second nearest neighbors. A comparison with the high-pressure data shows this softening to be anharmonic. A simple model relating the symmetry of the orbitals to that of the crystal structure is presented to explain the stiffness of the bonds between second nearest neighbors, while the decrease in the asphericity of the orbitals due to thermal electronic excitations is used to explain the discrepancy in the rate of softening with temperature.

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