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Temperature dependence of the phonon density of states in FeSi and CoSi. OLIVIER DELAIRE, Oak Ridge National Laboratory, MATTHEW LUCAS, MATTHEW STONE, DOUGLAS ABERNATHY — The phonon density of states (DOS) of the B20 compounds Fe(1-x)Co(x)-Si (x=0.0, 0.03, 0.5, 1.0) was measured as function of temperature from 10K to 773K using inelastic neutron scattering. The phonon DOS of FeSi exhibits an excess softening compared to the predictions of the quasiharmonic model, in agreement with previous measurements of elastic constants as function of temperature [1]. The phonon DOS of CoSi softens less, on the other hand, and appears in better agreement with the pure volume effect of the quasiharmonic model. These trends are compared to previous measurements of the temperature dependence of the phonon DOS in the A15 compounds V3Si and V3Ge [2]. Using first-principles electronic structure calculations, the observed anomalies are related to the details of the band structure in these compounds. It is shown that sharp features in proximity to the Fermi level lead to anomalous phonons through a sensitivity to thermal disorder, or adiabatic electron-phonon coupling. [1] D. Mandrus et al., Phys. Rev. B 51, 4763 (1994) [2] O. Delaire et al. , Phys. Rev. Lett. 101, 105504 (2008)

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