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Phonon Anomalies and Metal Insulator Transition in Fe(1-x)Co(x)Si OLIVIER DELAIRE, MATTHEW LUCAS, MATTHEW STONE, DOUGLAS ABERNATHY, KAROL MARTY, PAUL KENT, BRIAN SALES, DAVID MANDRUS, ORNL — The Fe(1-x)Co(x)-Si ordered compound (B20 structure) undergoes a metal-insulator transition upon doping with Co or heating. FeSi is a narrow band-gap semiconductor, whereas CoSi is a metal. Phonons were measured on both single crystals and powders as function of composition and temperature, using inelastic neutron scattering. A reciprocal-space time-of-flight tomography technique, as well as conventional triple-axis spectrometry, were used to map extensive regions of the FeSi dispersions. The phonon branches in FeSi exhibit an excess softening compared to those of CoSi, which appears in better agreement with a pure volume effect. Using first-principles electronic structure calculations and ab-initio molecular dynamics, the anomalies are explained in terms of a metallization induced by thermal disorder. This effect is also related to other cases where the electronic structure leads to anomalous temperature dependencies of the phonons.

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