Abstract Submitted
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Electron-phonon coupling in FeSi thermoelectrics: inelastic neutron scattering and first-principles simulations[1] OLIVIER DELAIRE, JIE MA, BRIAN SALES, PAUL KENT, MATTHEW STONE, KAROL MARTY, MATTHEW LUCAS, DOUGLAS ABERNATHY, DAVID MANDRUS, ORNL TEAM — FeSi is a promising thermoelectric material for refrigeration applications, with a Seebeck coefficient over 500μV/K at 40K. FeSi is a narrow band-gap semiconductor at low temperature (B20 structure), and undergoes a semiconductor-to-metal transition around room temperature. Using inelastic neutron scattering, phonons were measured on both single crystals and powders as a function of composition and temperature. We report a strong coupling between the phonons and the semiconductor-to-metal transition, upon increasing temperature and carrier concentration. Using first-principles electronic structure calculations and ab-initio molecular dynamics, we show that the band gap and the sharp features around the band edges are strongly affected by the thermal disordering induced by phonon excitations. We also report on the effect of heavy impurities (Ir, Os) on the phonons.

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