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(POS-16) Lattice Dynamical Study of High-Entropy Oxides

Tuesday, 7 June 2022 17:42 (2 minutes)

High-entropy oxides (HEOs) comprise an equimolar mixing of metal cations combined into a single-phase crystal structure. First synthesized in 2015 [1], HEOs have garnered much attention as candidates for high-efficiency batteries and heat shields [2, 3]. HEOs composed of four and five binary oxides have been previously investigated by infrared [4] and Raman spectroscopy [5] and lattice dynamical simulations. The IR spectra consist of a strong, reststrahlen mode at 350 cm^{-1} and a much weaker mode at 150 cm^{-1} not predicted by group theory. The absence of spin-phonon splitting in the reststrahlen band below the Neel temperature (T_N), despite appearing in the parent oxides CoO and NiO, has been attributed to a high rate of static disorder scattering. The Raman spectra are composed of five peaks which have been assigned to TO, LO, $LO + TO$, $2LO$ modes, as well as a two-magnon mode. Fits of the spectra to the Lorentz oscillator model revealed a temperature-dependent damping parameter which was ascribed to anharmonic effects. The phonon density of states will be simulated using GULP [6] in order to understand the IR and Raman spectra.

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