Canadian Association of Physicists
Association canadienne des physiciens et physiciennes

Contribution ID: **3757** Type: **Oral Competition (Graduate Student) / Compétition orale (Étudiant(e) du 2e ou 3e cycle)**

(G*) Vibrational Modes in High-Configurational-Entropy Rocksalt Oxides

Monday 19 June 2023 16:15 (15 minutes)

The high-entropy oxide (HEO) $Mg_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2}O$ is synthesized by annealing equimolar mixtures of the parent binary oxides MgO, CoO, CuO, NiO, and ZnO to 1000 K and quenching to 295 K. X-ray diffraction shows HEO crystallizes in a single-phase rocksalt structure. The cations randomly occupy the (000) site, while the oxygen sublattice is ordered. Lattice dynamical (LD) studies on amorphous Si (α-Si) have shown that structural disorder can induce localized phonon modes ('locons') beyond a high-frequency mobility edge in the vibrational density-of-states (VDOS). Locons are characterized by eigenvectors which decay exponentially and a participation ratio (PR) < 0.1. We have used the General Utility Lattice Program to study the optical properties and phonon localization in HEO. Previous LD studies on the elastic constants of ternary and quaternary oxides have obtained satisfactory agreement with experiment by neglecting cation-cation interactions and modelling cation-oxygen and oxygen-oxygen bonds with the Buckingham potential. Polarization effects are modelled using a shell model (SM) for oxygen; all cations are treated as point charges. In this work, we instead treat every atom with the SM: new Buckingham parameters for the binary oxides were obtained by fitting to experimental crystal structures, dielectric constants, and phonon frequencies. Agreement between the simulated VDOS and inelastic neutron scattering data is reasonable and improves upon existing models, which use a combination of the Buckingham potential and point charge approximation. Phonon mode localization was studied by calculating the PR of a 4096-atom supercell of HEO. Despite the strongly-disordered cation sublattice, it was determined that only of 0.5% modes are locons. This is roughly 10% of the number of locons in a similarly-sized cluster of α-Si. Furthermore, it was shown that the number of locons increases if sulfur atoms are randomly substituted into the oxygen sublattice.

Keyword-1

high-entropy oxide

Keyword-2

phonon localization

Keyword-3

lattice dynamics

Primary author: WILSON, Connor

Co-authors: CRANDLES, David (Brock University); Dr GANESH, Ramachandran (Brock University); Dr AFSHARVOSOUGHI, Tahereh (Brock University)

Presenter: WILSON, Connor

Session Classification: (DCMMP) M3-8 Materials Physics | Physique des matériaux (DPMCM)

Track Classification: Technical Sessions / Sessions techniques: Condensed Matter and Materials Physics / Physique de la matière condensée et matériaux (DCMMP-DPMCM)