Materials Science & Engineering Graduate Seminar

Wednesday, Septemer 4 2019, 4:10-5:00PM, WEB 1230

Mahsa Ebrahiminia

PhD candidate, Materials Science & Engineering

Structural, Mechanical, and Dynamical Properties of Amorphous Li2CO3 from Molecular Dynamics Simulations

Advancement in alternative energy technologies and environmental concerns with utilization of limited fossil resources bring a growing demand for the improvements of energy storage devices. Lithium ion batteries have been widely used in many areas that necessitate improvements in their safety and efficiency, which in turn requires more detailed understandings of its structure. Li2CO3 is one of the main components in the electrode/electrolyte interface that plays an important role in defining the performance of batteries.
Structural, mechanical, and transport properties of amorphous Li2CO3 were studied using MD simulations over a wide temperature range. At higher temperatures, both anion and cation diffusion coefficients showed similar temperature dependence. However, below Tg, the anions formed a glassy matrix, while Li+ continued to be mobile. The conductivity of Li+ at room temperature was estimated to be on the order of 10-6 S/cm. Mechanical analysis revealed that the shear modulus was high enough to suppress dendrite growth.

Marcus Parry

PhD candidate, Materials Science & Engineering

Lattice strain, texture development, and incompressibility of superhard Mo0.9W1.1BC and ReWC0.8

Superhard materials, classified by a Vickers hardness exceeding 40 GPa, are utilized in a variety of applications including cutting, grinding, drilling, as well as in automotive, aerospace, and defense industries. To expedite the discovery process of novel superhard compositions, a machine-learning (ML) model is developed to predict bulk and shear moduli; elastic properties which scale with hardness. From the model, Mo0.9W1.1BC and ReWC0.8 compositions are selected and synthesized via arc melting. Bulk modulus of each compound is determined through hydrostatic diamond anvil cell (DAC) compression experiments, corroborating the ML predictions within 10% error. Indentation experiments reveal each composition exceeds the superhard threshold at low loads. Furthermore, hardening mechanisms and anisotropic deformation behavior are elucidated via nonhydrostatic DAC experiments by comparatively assessing lattice strain and texture development in Mo0.9W1.1BC and ReWC0.8. Utilization of predictive ML algorithms and developing correlations among structural, elastic, and mechanical properties benefits future design of superhard materials.