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LAMMPS Simulations of Ternary CuTiZr Metallic Glasses[1]
SARA CHENG, University of California Berkeley, LEV GELB, University of Texas Dallas — Metallic glasses are a family of amorphous solids which display highly desirable material properties. These include high magnetic permeability, high hardness, and absence of micro structures such as grains and phase boundaries (Miller 2011). In this computational study we apply a three-step heating treatment to a ternary mixture of copper, titanium, and zirconium to study glass formation and recrystallization. We empirically apply a Second Moment Approximation Tight Binding Potential with adjustable parameters, outlined in Dalgic *et al.* (2011), Qin *et al.* (2011), and Rosato *et al.* (1993). We calculate the temperature, volume, pressure, and total energy of the system as functions of simulation time. We also calculate the radial distribution function for the entire system as well as grouped atom constituents. We employ common neighbor analysis to qualify the structure of clusters of atoms in terms of either face-centered-cubic, hexagonal close packed, icosahedral, or unknown configurations.

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