Abstract

Multi-component High Entropy Alloys (HEAs) have opened a plethora of opportunities in achieving superior properties to traditional alloys owing to several well-established theories. Viscoelasticity is defined as the ability of the material to store and dissipate energy as a time-dependent phenomenon that has several applications starting from noise reduction, sound attenuation, high-frequency damping in a mechanical resonator, optoelectronics, ferroelectrics, etc. Recent research has brought a lot of attention to viscoelastic damping in crystalline materials; however, damping in HEAs have hitherto remained unexplored, which forms the focus of this work. HEAs offer high stiffness, and mechanisms for viscous damping (via formation of solid solutions and defects), that, when combined, offers promise for significant viscoelastic damping.

Here, we use molecular dynamics simulations to perform oscillatory shear deformations to study the frequency-dependent viscoelastic damping in model FeNiCrCoCu HEA, in the frequency range from 0.01 to 1 THz. We evaluate the loss modulus from the time-dependent stress-strain data and correlate mechanisms of damping with various conditions such as the temperature, shear rate, and amplitude of shear deformation. Correlations between the high-frequency shear response with the vibrational states of defect-free and defected HEAs are made. Notably, we show that defects such as vacancies, dislocations and stacking faults play an important role in the damping mechanism and can be modulated for optimum damping performance. The viscoelastic behaviour is further confirmed and correlated with phonon calculations exhibiting anharmonic phonon-phonon coupling to be the dominant phenomenon responsible for large damping.

Keywords: High Entropy Alloys, Viscoelasticity, Loss Modulus, Vacancies, Dislocations, Stacking Fault