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Atomistic investigation of grain boundary triple junctions energetic in face centered cubic materials

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ABSTRACT

Triple junctions (TJs) constitute a large volume fraction of nanocrystalline materials and its properties have been found to be very different than that of their constituent grain boundaries. Furthermore, the TJs play an important role in determining material properties, such as solute segregation, grain growth, and plastic deformations. In this study, the structural stability of various TJs formed by the intersection of <110> symmetric tilt grain boundaries in FCC materials (Al, Cu, and Ni) were investigated using molecular statics. Continuum measures such as the net change in volume, the excess energies, the resolved surface tensions, and the resolved line tensions were calculated due to the formation of TJ. Comparing the line tension and excess energies for each TJ shows that the normalized excess energies of all three FCC metals are comparable and the line tension trend follows that of the elastic anisotropy, i.e., Cu TJs have the highest line tension followed by Ni and Al. Furthermore, the secondary objective of this study was to understand the atomistic relationship between the local structure and the point-defect (vacancy) energetics at the TJs and their constituent GBs. Toward this, we performed detailed atomistic characterization of TJs energetics and then evaluated vacancy binding energy at the TJs. The simulation results revealed that the TJ local arrangements and resulting structural units have a significant influence on the magnitude of vacancy binding energies, and the site-to-site variation within the TJ is substantial. This is significant for applications where extreme environmental damage generates lattice defects, TJs and their constituent grain boundaries act as sinks for both vacancies and interstitial atoms.