Prdiction of mechanical property of Ni-Al nanopowder via coarse-grained simulation

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Reactive nanocomposites are utilized for many applications. In particular, Ni-Al nanocomposites have been widely studied for its extreme reactivity and chemical stability. In this theoretical study, we estimated the mechanical properties of Ni-Al nanocomposites in the form of nanopowder using coarse-grained simulation based on molecular dynamics (CGMD). First, coarse-grained beads were modeled to have a few nanometer size and their interaction parameters were derived from embedded atom method (EAM) potentials. Subsequently, model systems of Ni-Al nanopowder were built and equilibrated with CGMD at standard temperature and pressure. Elastic modulus of each model system were statistically measured and stress-strain relations were obtained by dynamic monitoring of uniaxial compression and extension in the elastic region. For this calculation, different morphologies such as amorphous and lamellar were probed with size variation of each Ni and Al bead. Our model system covers wide length scale from tens of nm level to a few μm level to investigate the size effect of nanoparticles on mechanical properties.