Prediction of EOS and Elastic modulus of Ni/Al nanopowder and nanofoil by Molecular Dynamics

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There are numerous studies regarding Ni/Al alloy for its extreme reactivity, which can be used for various applications, but not in the forms of nanopowder and nanofoil. Thus, we have obtained the equation of state and elastic modulus of Ni/Al alloy in those structures. We have made various model systems to check the equation of state of each material (i.e. Ni and Al) and elastic modulus at different conditions (e.g. stoichiometric ratio and nanocluster size for 'nanopowder', layer thickness and layer frequency for 'nanofoil' at different temperature and pressure). We employed classical Molecular Dynamics (MD) with Modified Embedded-Atom Method (MEAM) Potential, of which parameters are based on thermal and mechanical properties. Furthermore, through Coarse-Grained Molecular Dynamics (CGMD), the behavior of phase changes of those structures was investigated in terms of size.