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Modeling and Simulation of the Structural, Electronic and Magnetic Properties of Fe-Ni Based Nanoalloys

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Abstract : There is a growing interest in the modeling and simulation of magnetic nanoalloys by various computational methods. Magnetic crystalline/amorphous nanoparticles (NP) are interesting materials from both the applied and fundamental points of view, as their properties differ from those of bulk materials and are essential for advanced applications such as high-performance permanent magnets, high-density magnetic recording media, drug carriers, sensors in biomedical technology, etc. As an important magnetic material, Fe-Ni based nanoalloys have promising applications in the chemical industry (catalysis, battery), aerospace and stealth industry (radar absorbing material, jet engine alloys), magnetic biomedical applications (drug delivery, magnetic resonance imaging, biosensor) and computer hardware industry (data storage). The physical and chemical properties of the nanoalloys depend not only on the particle or crystallite size but also on composition and atomic ordering. Therefore, computer modeling is an essential tool to predict structural, electronic, magnetic and optical behavior at atomistic levels and consequently reduce the time for designing and development of new materials with novel/enhanced properties. Although first-principles quantum mechanical methods provide the most accurate results, they require huge computational effort to solve the Schrodinger equation for only a few tens of atoms. On the other hand, molecular dynamics method with appropriate empirical or semi-empirical inter-atomic potentials can give accurate results for the static and dynamic properties of larger systems in a short span of time. In this study, structural evolutions, magnetic and electronic properties of Fe-Ni based nanoalloys have been studied by using molecular dynamics (MD) method in Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) and Density Functional Theory (DFT) in the Vienna Ab initio Simulation Package (VASP). The effects of particle size (in 2-10 nm particle size range) and temperature (300-1500 K) on stability and structural evolutions of amorphous and crystalline Fe-Ni bulk/nanoalloys have been investigated by combining molecular dynamic (MD) simulation method with Embedded Atom Model (EAM). EAM is applicable for the Fe-Ni based bimetallic systems because it considers both the pairwise interatomic interaction potentials and electron densities. Structural evolution of Fe-Ni bulk and nanoparticles (NPs) have been studied by calculation of radial distribution functions (RDF), interatomic distances, coordination number, core-to-surface concentration profiles as well as Voronoi analysis and surface energy dependences on temperature and particle size. Moreover, spin-polarized DFT calculations were performed by using a plane-wave basis set with generalized gradient approximation (GGA) exchange and correlation effects in the VASP-MedeA package to predict magnetic and electronic properties of the Fe-Ni based alloys in bulk and nanostructured phases. The result of theoretical modeling and simulations for the structural evolutions, magnetic and electronic properties of Fe-Ni based nanostructured alloys were compared with experimental and other theoretical results published in the literature.

Keywords : density functional theory, embedded atom model, Fe-Ni systems, molecular dynamics, nanoalloys
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