Molecular Dynamics Simulations of Fe-Pt Nanoparticles

Jayendra Balasubramanian, Dale Vickery, John Wiest

Dept. of Chemical and Biological Engineering
The University of Alabama

Abstract

Molecular Dynamics Simulations are used to understand structural and thermodynamic properties of FePt nanoparticles. These simulations can give us a wealth of information about the crystal structure and ordering of FePt nanoparticles and predict structural changes and thermodynamic behaviour at under a variety of conditions such as changing temperature and sintering.

Newton’s 2nd Law for atom i:

\[ m_i \frac{d^2 \mathbf{r}_i}{dt^2} = -\mathbf{F}_i = \mathbf{F}_{\text{external}}(\mathbf{r}_i) + \mathbf{F}_{\text{inter}}(\mathbf{r}_i) + \mathbf{F}_{\text{emb}}(\mathbf{r}_i) \]

Interatomic Forces:

\[ \mathbf{F}_{\text{inter}}(\mathbf{r}_{ij}) = \sum_{j \neq i} \mathbf{F}_{\text{emb}}(\mathbf{r}_{ij}) + \mathbf{F}_{\text{potential}}(\mathbf{r}_{ij}) \]

Embedded Atom Potentials

\[ E = \frac{1}{2} \sum_i \sum_{j \neq i} \phi_{ij}(\mathbf{r}_{ij}) + \sum_i F_i(\rho_i) \]

\[ \rho_i = \sum_j f_j(\mathbf{r}_{ij}) \]

\[ \phi_{ij} = \text{Pair Potential} \]

\[ F_i = \text{Embedding Energy} \]

\[ \rho_i = \text{Local Electron Density} \]

\[ f_j = \text{Electron Density Function} \]

Pair Interactions + Embedding Energy

Alloy Model- The Johnson EAM Potential

\[ E = \frac{1}{2} \sum_{j \neq i} \phi_{ij}(\mathbf{r}_{ij}) + \sum_i F_i(\rho_i) \]

\[ \rho_i = \sum_j f_j(\mathbf{r}_{ij}) \]

\[ \phi_{ij}(\mathbf{r}_{ij}) = \frac{1}{2} \left( \frac{f'_i(\mathbf{r}_{ij})}{f'_i(\mathbf{r}_{ij})} \mathbf{r}_{ij}^2 + \frac{f''_i(\mathbf{r}_{ij})}{f''_i(\mathbf{r}_{ij})} \mathbf{r}_{ij}^4 \right) \]

EAM Potential will allow us to simulate alloy metal systems.

- FePt and FePtx magnetic nanoparticles for ultra high density data storage.
- Bimetallic and trimetallic nanoparticles for catalysis.

Future Work

- Simulate particles with defects in the crystal structure
- Simulate FePtX trimetallic nanoparticles and study the effects of a third element on phase transition and ordering
- Determination of an order parameter from fourier transform analyses to examine the degree of ordering at various temperatures
- Study the effect of size of particles on the stability of the L10 phase and phase transition.