Effects of size, shape and structure on the Curie temperature of Fe and Ni nanoparticles

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Introduction

Magnetic nanoparticles used for data storage tend to get smaller and smaller, in order to increase the density of stored data and reduce the size of devices [1]. Therefore, studies of effects of finite size on these small nanoparticles is of utmost importance to understand the physics that governs them. An atomistic approach is the most suitable for this class of studies, where the fluctuations of the lattice and the real atomic structure is taken into account to study the magnetic properties [2]. In this work, we use a combination of molecular dynamics and atomistic spin models to investigate the effects of size, shape and lattice fluctuations on the magnetic properties of Fe and Ni nanoparticles. This effects are found to contribute to a change in Curie temperature.

Modelling methods

The atomic structures of small Fe and Ni nanoparticles are simulated using molecular dynamics. The magnetic properties are simulated using a spin classical Hamiltonian:

$$H = -\sum_{i \neq j}^{N} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \qquad (1)$$

taking into account the long-range nature and the dependence of the atomic separation of the exchange interaction [3]. The time evolution of magnetization is calculated using the numerical solution of the Landau Liftshitz-Gilbert equation and the Langevin dynamics [4].

$$\frac{\partial \mathbf{S}_i}{\partial t} = -\frac{\gamma}{(1+\lambda^2)}[\mathbf{S}_i \times \mathbf{H}^i_{eff} + \lambda \mathbf{S}_i \times (\mathbf{S}_i \times \mathbf{H}^i_{eff})] \qquad (2)$$

Conclusions

- Simulated microstructures show the expected faceting which gives a large difference in the predicted magnetic properties when compared with ideal shapes such as cubic and spherical particles.
- The results suggest that to study the magnetic properties of small nanoparticles a realistic structure and shape should be used.
- A persistent ferromagnetic ordering above the Curie temperature is observed due to the effects of size.

References

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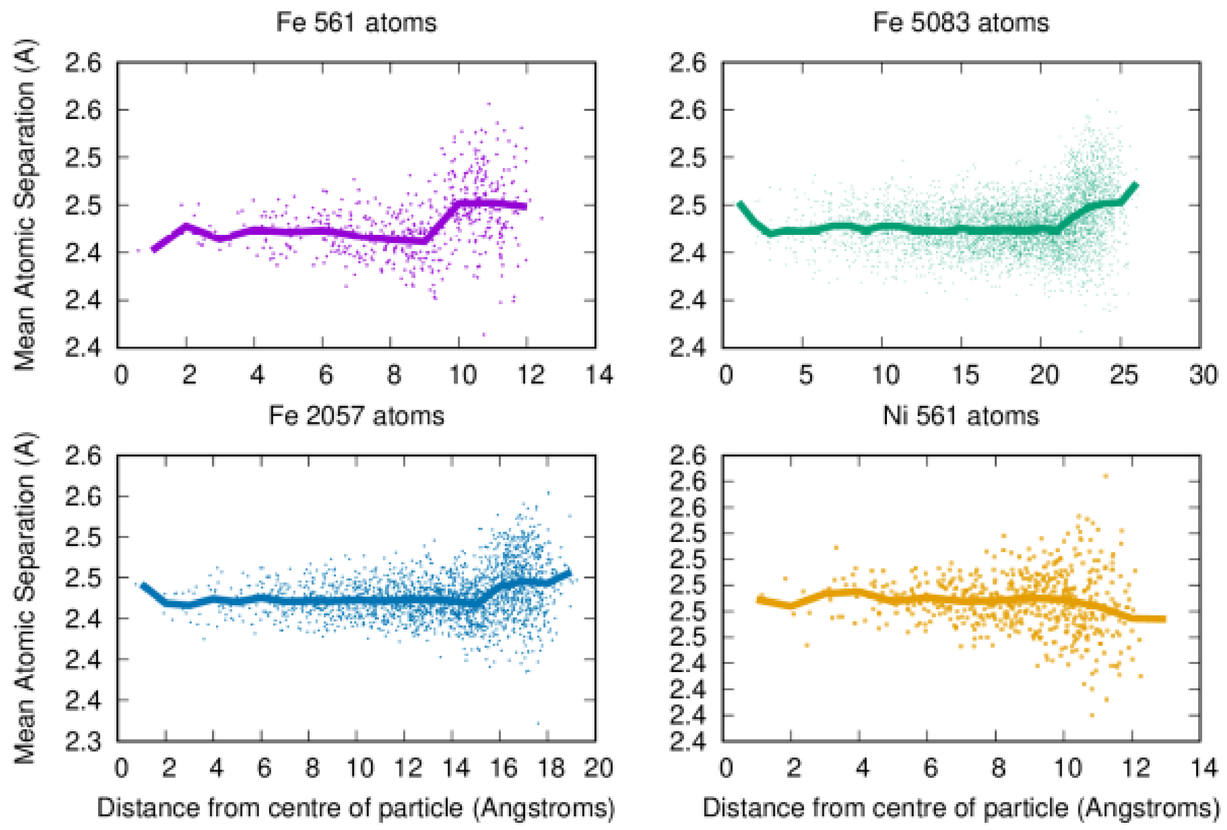
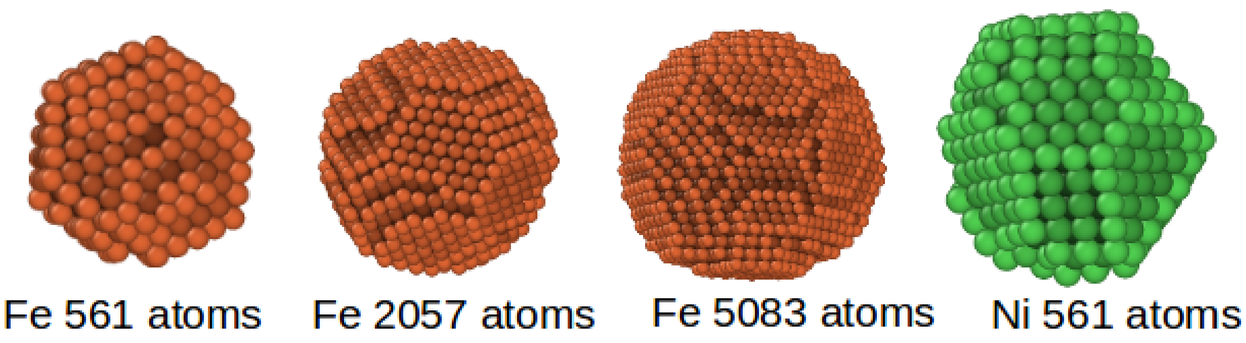
Structural Analysis

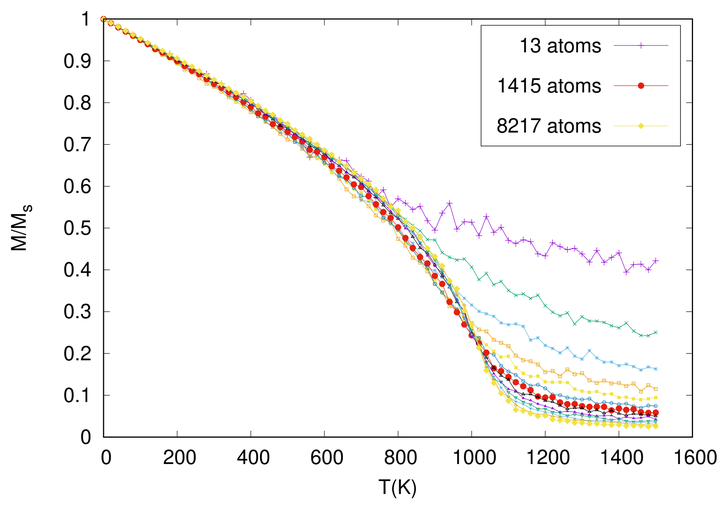
Graphs show the mean interatomic separation as a function of the radial distance from the center for the Fe and Ni particles. The lines represent the weighted average of the points. The extent of the scattering in the mean atomic spacing is clearly noted as a result of thermal fluctuations. These dispersions can significantly affect the Curie temperature of these particles, since the exchange energy varies greatly with interatomic separation.

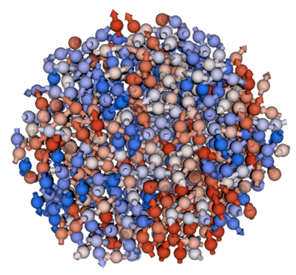




Results

The graph shows the size dependence of the Curie temperature for nanoparticles de Fe. It is





The plots show the dependence of the shape of the Curie temperature. It is observed that the molecular dynamics particle has a higher Curie temperature than the spherical and cubic particle.