EP02

Shell-wise Ferrimagnetic Properties of Free Iron Icosahedral Clusters from Ab *initio* Calculations

Zhida Cheng, Tao Ling, and Jing Zhu*

Beijing National Center for Electron Microscopy, Tsinghua University, Beijing 100084, China.
Laboratory of Advanced Materials, Department of Materials Science and Engineering,
Tsinghua University, Beijing 100084, China.

*Corresponding author: e-mail: jzhu@mail.tsinghua.edu.cn

Magnetic properties of transition metal clusters have been intensively investigated by theoretical and experimental methods due to the interest in unusual behavior introduced by surface effect and the quantum effect at nanoscale. Previous work on free iron clusters with bulk structures have been researched by molecular dynamics [1] and *ab initio* calculations [2].

Recently, freestanding iron clusters with icosahedral symmetry have been successfully synthesized and identified with high-resolution TEM (HRTEM) in our research group. In order to predict and explain the properties of the products, we performed calculations using the siesta package [3]. GGA and LDA schemes for the exchange and correlation potential were used in our work, respectively. The structures of the iron clusters have been fully relaxed to represent more reasonable results.

First, we studied ferromagnetic properties of icosahedral clusters containing different numbers of atoms. In each cluster, the atom located at the center has unusually small magnetic moment, while the magnetic moments of surface atoms are increased. The results are in good agreement with the reference [4].

Besides the ferromagnetic and nonmagnetic configuration, a shell-wise ferrimagnetic order for Fe_{55} icosahedron cluster was found for the first time in our calculation. The magnetic moments of the surface atoms are as large as ~2.4 μB (green) and ~3.1 μB (blue), respectively. The center atom (yellow) with smaller magnetic moment (~ -0.66 μB) has a different spin direction from those of surface atoms. Also, the atoms in the second shell (red) have interestingly small magnetic moments (~ -0.15 μB) with the identical direction to the center atom. This configuration can be achieved spontaneously from relaxation of a nonmagnetic state but is metastable in external magnetic field.

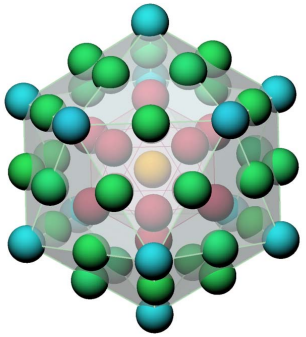

Fig. 1. Structure of ferrimagnetic icosahedral iron cluster.

This work is financial supported by National 973 Project of China, Chinese National Nature Science Foundation.

REFERENCES

[1] P. Ballone et al., Chem. Phys. Lett. 233, 632 (1995).
[2] S. Polesya et al., Europhys. Lett., 74 (6) 1074-1080 (2006).
[3] José M Soler et al., J. Phys.: Condens. Matter 14, 2745-2779 (2002).
[4] A.V. Postnikov et al., Eur. Phys. J. D 25, 261-270 (2003).

EP03

Magnetism and Magnetocrystalline Anisotropy in Tetragonally Distorted γ-Fe (001) Surface

Won Seok Yun, Gi-Beom Cha, and Soon Cheol Hong*

Department of Physics, University of Ulsan, Ulsan 680-749, South Korea

*Corresponding author: e-mail: schong@mail.ulsan.ac.kr

Magnetic thin films exhibit significantly different magnetic properties from their bulks, such as magnetocrystalline anisotropy (MCA), enhanced magnetic moments, and critical behaviors. These differences are caused by the increasing influence of the reduced dimensionality and by the strain induced by the epitaxial constraint at the interface. In the bulk, α-Fe is ferromagnetic (FM) and metastable γ-Fe can exist in various magnetic states of paramagnetic (PM), antiferromagnetic (AFM), FM, and spin-spiral states, depending on the lattice constant and the lattice distortion. It was reported that γ-Fe can be stabilized by epitaxial growth on appropriate substrate such as Cu (001) or Cu (111) at low temperature.

Recently first principles calculations on fcc-based bulk Fe showed its complex magnetic structure [1]. The bulk γ-Fe in AFM state was found to accompany tetragonal distortion and was more stable compared to a high spin (HS) FM state which was stabilized in a cubic symmetry. Even though an AFM state is most stable as expected, the energy difference between AFM and HS FM states was calculated to be quite small (about 20 meV). Hence, it would be a quite interesting question what are the most stable magnetic state at a surface and how far below the surface magnetism are affected. Thickness dependence of the magnetic anisotropy of a pure γ-Fe film has not been studied in detail yet.

In this work, we have carried out extensive studies the correlation between magnetism and atomic structure of γ-Fe (001) surfaces, using the highly precise full-potential linearized augmented plane-wave (FLAPW) method based on generalized gradient approximation (GGA). In order to take surface and size effects into account, the tetragonally distorted γ-Fe films with different thickness were simulated by single slabs. We used a equilibrium lattice constant (3.49 Å) [1] of bulk tetragonally distorted γ-Fe for AFM state as the in-plane lattice constant. The total energies of Fe thin films composed of 3-, 5-, 7-, 9-, and 11-layers for possible different collinear spin configurations were calculated.

As a result, the magnetic state of FM coupling between two adjacent Fe layers at the surface and AFM coupling between the rest inner layers was found to be most stable, not depending on the film thickness. The MCA energies of the systems were calculated by using a torque method. It was proved that the spin orientations of the systems are perpendicular to the surface regardless of their thickness. The calculated total magnetic moment of a Fe atom at the surface was found to be significantly enhanced to about 2.70 μ_B compare d to the tetragonally distorted bulk γ-Fe (1.63 μ_B). Detailed discussion on the origin of ferromagnetism at the surface will be discussed in the conference.

REFERENCES

[1] D. Lee and S.C. Hong, J. of Magnetics 12, 68 (2007).