Ab Initio Calculation on Magnetism of Monatomic Fe Nanowire on Au (111) Surface

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Abstract. The magnetic anisotropy of the one-dimensional monatomic Fe wire on the Au (111) texture has been theoretically analyzed using Wien2k framework. The model simulates experimentally observed ferromagnetic Fe monatomic wire self-organized along the terrace edge of the Au (788) plane, which exhibits the magnetization perpendicular both the wire and Au plane. In the case of the model consisting the one-dimensional Fe wire placed on the Au (111) plane with the Au lattice cite, no significant anisotropy is resulted by the calculation. On the other hand, the model where the Fe wire is formed along the Au terrace like step indicates the anisotropy of which easy direction is along the wire, resulting in different direction from the experiment. When we introduce the disorder in the Fe wire array, the easy direction changes. As for the model that the every other Fe atoms are slightly closer to the Au step (≈ 0.0091 nm) the easy direction turns to be perpendicular to the wire and parallel to the Au plane, that is, the dislocation direction. The disorder in the Fe wire seems to play significant roll in the anisotropy.

1. Introduction
It is known through theoretical analysis that the one-dimensional atom array shall not be ferromagnetic. However several reports revealed that slightly disordered monatomic atom array might have ferromagnetic ground state [1]-[3]. In the experimental works the ferromagnetism is confirmed for one-dimensional Co wire which is self assembled on the Pt (997) plane [4]. Before this work several researches were carried out on the ferromagnetism of nanometer sized structure formed using steps in the (11n) plane [5, 6]. Since then energetic researches are made in one-dimensional monatomic wires. Among them the ferromagnetism in Fe monatomic wire formed on Au (111) plane was confirmed using angle-resolved photoemission spectroscopy [7] and also the same group that the magnetic easy direction of the Fe monatomic wire self organized on the terrace edge of Au (788) plane becomes perpendicular to both the wire and Au plane [8]. In addition Spišák and Hafner carried out ab initio calculation on the Fe monatomic wire on the Cu (11n) plane and concluded that Fe becomes ferromagnetic and its Curie temperature is between 200 and 300 K [9]. Tight binding calculation is also applied to monatomic wire [10] and it revealed that the orbital momentum of the d electrons plays an important roll for magnetic anisotropy in the wire structure.

In this work we have carried out ab initio calculation on the monatomic Fe wire with small disorder on the Au (111) surface and examined the magnetic anisotropy of the Fe wire formed at Au step edge.
Figure 1. Calculation models of Fe nanowire. (a) Fe wire on Au (111) plane, (b) Fe wire at the step edge of Au (111) and (c) Fe wire at step edge with slight dislocation.

2. Models and calculation
The models of one-dimensional monatomic Fe wire formed on Au (111) plane or at the edge are shown in Fig.1. We prepared 3 types of the model structures. A simple structure of the Fe wire (a) is on the fcc Au (111) monatomic layer. The lattice constant of the Au underlayer is the same as that of the bulk Au ($a=0.40786$ nm). Fig.1 (a) is the top view of the model and the wires run horizontally. Fe atoms are located in the weight center position of the triangle formed by Au atoms. The height of the Fe atom is 0.2104 nm from the Au plane center and it is selected so that the total energy of the system takes minimum. The distance between the Fe atoms is same as that of the Au atoms. Hence the Fe wire is extended toward the wire axis compared with original Fe lattice constant. The second model (b) consists of the Au plane with Au steps of which height is one monolayer. Fe atoms are put on the lattice position near the step edge. The height of the Fe atoms are same as that in the model (a). And the third model (c) has slight dislocation in Fe position. Planar position of the every other Fe is shifted toward the edge by 0.0091 nm, which is a half distance of the spacing between the Fe and Au arrays. This introduces disorder in Fe wire in one direction.

Ab initio calculation is carried out using FLAPW based Wien2k framework[11]. GGA potential[12] is used. Calculation admits the spin polarization in every cases. Spin-orbit coupling is introduced in the calculation. We examined the magnetic anisotropy comparing the energies resulting from various magnetization axis in the Fe wires.

3. Results and Discussion
3.1. Simple wire model
Three kinds of the magnetization (M) direction (M//wire, M//Au plane ($\perp$wire) and M$\perp$Au plane) are considered in the calculation incorporating the spin-orbit coupling. Comparison of the system energies between these configurations is listed in Table 1. The values of the energies indicate differences of the total system energy from the energy in case of magnetization parallel with the wire axis. In the present configuration the energy minimum occurs for magnetization perpendicular both to the wire and Au plane. But the energy differences are very small as 0.0001–0.0002 Ry and these values are close to the energy conversion criteria of 0.0001 Ry for this calculation. We should not say that this configuration has significant magnetic anisotropy.

3.2. Model of Fe wire at Au step edge
In order to make the model more realistic one where Fe wire is formed on the Au (788) terrace edges, we made the atomic step on the Au (111) plane. The Au step runs linearly on the Au (111) plane being located at the lattice position. Fe atoms are placed also the lattice position of
Table 1. Energy difference in magnetization direction for various wire models.

| Direction      | Simple wire | Wire at step edge | Wire with dislocation |
|----------------|-------------|-------------------|-----------------------|
| M // wire      | 0           | 0                 | 0                     |
| M // Au plane  | -0.000113   | 0.002526          | -0.002073             |
| M ⊥ Au plane   | -0.000218   | 0.002379          | -0.001574             |

the center of Au triangle but this time the Au atoms are also placed aside at the same height. The results of the energy calculation is listed in the middle column of Table 1.

In this case the magnetization easy axis turns to the wire axis direction and the differences are increased by one order compared to the previous model. Hence the energy difference seems to be significant in this configuration.

3.3. Model of Fe wire with slight dislocation

In the real system it is considered that the Fe atoms consisting wires are not imposed to the place with the Au lattice positions, that is, Fe wires consist of Fe atoms bound with each other and the wire located at the Au terrace edge. Hence the Fe wire is not a straight linear structure but zig-zagged arrangement of the Fe atoms along with the shape of the Au atom plane. Therefore we have prepared another model that includes Fe atom dislocation. As a first step we put Fe atoms so that the wire forms zig-zag line. The amount of dislocation is 0.0091 nm and the direction is parallel to the Au plane.

The results of the energy difference listed in the right column of Table 1 indicate that the easy axis is perpendicular to the wire and parallel to the Au plane, resulting in the different anisotropy with the experiment [8]. The densities of states (DOS) are also calculated for the Fe wire at the Au edge models. Fig. 2 shows the DOS of the d electrons for (a) straight wire and (b) disordered wire. The value of dislocation is not so large, but the DOS’s differ significantly. Low dimensionality causes large splitting and spiky shape in the DOS. In both models d states

Figure 2. Densities of states in Fe wire on the edge models. (a) Straight wire and (b) disordered wire model.
split into 5 orbitals and it is quite different from the bulk where \( d \) orbital momentum quenches. In the straight wire (a) the average energy of \( d\gamma \) (\( 2z^2 - x^2 - y^2 \) and \( x^2 - y^2 \)) and \( d\varepsilon \) (\( 2xy, 2yz \) and \( 2xz \)) orbitals of up spin are -2.64 and -2.56 [eV], respectively. On the other hand in the model with disorder they become -3.32 and -2.77 [eV]. Although at present we have no concrete idea how this difference in the band structure affects on the origin of the easy direction change with Fe atom dislocation, this change in the band structure such as deeper \( d\gamma \) state in the disordered model may affect the magnetic anisotropy. We might need further analysis such that the dislocation direction is perpendicular to the Au plane or parallel to the wire in the future.

4. Conclusion
The theoretical analysis on the magnetic anisotropy of the one-dimensional monatomic Fe wire on the Au (111) texture calculated using Wien2k framework was discussed. Three types of the models, Fe wire on the Au (111) plane, Fe wire along the Au step on the (111) plane and the Fe wire including slight dislocation, are examined. Spin-orbit coupling is incorporated in the calculation so that the magnetic easy direction is obtained through system energy difference. In the case of the model consisting the one-dimensional Fe wire placed on the Au (111) plane with the Au lattice cite, no significant anisotropy was resulted by the calculation. On the other hand, the model where the Fe wire is formed along the Au terrace like step indicated the anisotropy of which easy direction is along the wire, resulting in different direction from the experiment. When we introduced the disorder in the Fe wire array, the easy direction changed. As for the model that the every other Fe atoms were slightly closer to the Au step (≈ 0.0091 nm) the easy direction turned to be perpendicular to the wire and parallel to the Au plane, that is, the dislocation direction. The disorder in the Fe wire seems to play significant roll in the anisotropy.

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