S-7

Electronic Structures and Magnetism of Fe-Co Binary Nanowires

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1. Introduction

Ferromagnetic nanowires and their arrays have attracted a great deal of interest because of their potential applications in magnetic sensors, memory devices, spintronic nanodevices, and energy storage [1,2]. In particular, Fe-rich nanowire alloys are widely used in order to control the magnetic properties of recording media by adjusting the concentration. Recently, the freestanding Fe-Co and Fe-Cr nanocluster wire (NCW) bundles were synthesized by a simple fabrication method using a resistive heater placed in the middle of a pair of permanent disk magnets [3]. In this work, we investigated the possible structures and the magnetic properties of freestanding Fe-Co nanowires for some Co concentration. Spin polarized *ab initio* calculations are performed in order to consider magnetism. The variation of spin polarizations for freestanding Fe-Co nanowires are demonstrated with relation to magnetoresistance ratio. We obtain the coercivity using the chain-of-spheres model with symmetric fanning mechanisms and compare with the experimental coercivity [4,5].

2. Model and computational method

We have used freestanding and infinite $Fe_{(1-x)}Co_x$ nanowires with centered-staggered triangle and square structures. The axis of wire is taken along z-axis and the lattice parameters of unit cell in xy-plane are set as 20 Å. The structures of $Fe_{(1-x)}Co_x$ nanowires are fully relaxed for a variety of Co concentration. The first-principles total energy and electronic structure calculations have been carried out within the generalized gradient approximation of Perdew-Wang 1991 with Vosko-Wilk-Nusair spin interpolation for the exchange-correlation energy using the ultrasoft pseudopotential plane wave method and projector augmented wave potentials. The energy cutoff of the plane wave basis set is taken to be 270 eV and the total energies of nanowires are converged to 10^{-3} eV. We have used 2 × 2 × 10 k-points in Monkhorst-Pack scheme and optimized geometries until the atomic force is less than 0.01 eV/Å.

3. Results and discussion

We compared the calculated lattice constants of Fe-Co nanowires with experimental results [3], as given in Fig. 1. The calculated lattice constants of Fe-Co nanowires with centered-staggered square structure are slightly longer than experimental values and suddenly drop down at x = 0.3. The experimental lattice constants also suddenly decreased at x = 0.2 and slowly increased with increasing Co component [3], while the calculated values for bcc Fe-Co bulks gradually go down from x = 0.5. We found that there is an important common feature that the lattice constants below x = 0.25,

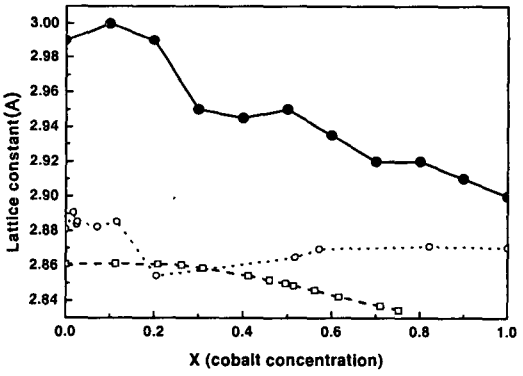

Fig. 1. The lattice constants of $Fe_{(1-x)}Co_x$ nanowires with centered-staggered square structure (filled circle). The experimental results of freestanding Fe-Co nanowires with bcc structure are shown by open circle [3] and the calculated values for bcc Fe-Co bulk alloys at room temperature are indicated by open square.

Fe-rich Fe-Co nanowires, are longer than those in other Co concentration.

We have obtained the magnetic moments of Fe-Co nanowires with centered-staggered triangle and square structures, as displayed in Fig. 2. We show that the magnetic moments are much dependent on the Co concentration regardless of nanowire shape. The Slater-Pauling curve presents a peak near x = 0.35 and rapidly drops down at x = 0.8, where the Fe-Co bulk alloys change from bcc to fcc structure. While our calculated magnetic moments of Fe-Co nanowires have the highest value near x = 0.25 and gradually decrease with increasing Co concentration. The calculated magnetic moments of Fe-rich Fe-Co nanowires below x = 0.3 are 15 % larger than experimental values. However, the whole trend of magnetic moments is similar to that of Fe-Co bulk alloys with geometrical evolution from bcc to fcc structure.

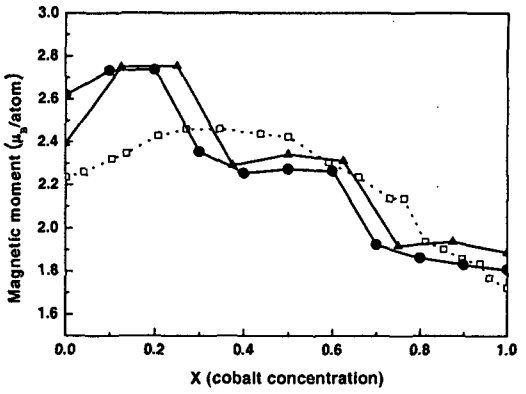

Fig. 2. The magnetic moments of $Fe_{(1-x)}Co_x$ nanowires with centered-staggered triangle (filled triangle) and square structure (filled circle). Open square denotes Slater-Pauling curve.

The chain-of-spheres model was proposed to understand the magnetization reversal process for magnetic nanowires, which is considered to be a chain of single domain spheres with uniaxial magnetic anisotropy [4]. Zhan *et al.* used the aspect ratio (length/area; $n \approx 375$) of nanowire fabricated in porous anodic alumina templates [4]. We set the slightly larger value which is 400 enough to present an infinite nanowire. Figure 3 shows the calculated coercivity of $Fe_{(1-x)}Co_x$ nanowires using the chain-of-spheres model with symmetric fanning and parallel rotation magnetization reversal mechanism. The trend of coercivity obtained by symmetric fanning mechanism agrees well with the experimental results of nanowire arrays inserted in porous templates, although the coercivity of pure Co nanowire is slightly higher than the experimental value because no structural transformation to fcc structure has been occurred. We find the freestanding Fe-Co nanowires have high coercivity like as the nanowire arrays combined in porous templates. This result suggests the freestanding Fe-Co nanowire bundles fabricated without templates are promising candidates for high-density magnetic recording media.

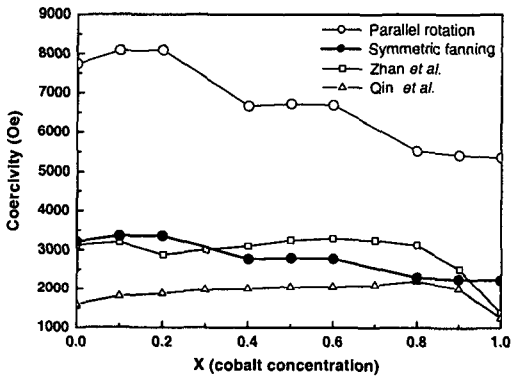

Fig. 3. The calculated coercivity of $Fe_{(1-x)}Co_x$ nanowires as a function of Co concentration using the chains-of-spheres model in parallel rotation (open circle) and symmetric fanning (filled circle) mechanism.

4. Reference

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