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Structural and Magnetic Properties of Epitaxial Fe_xCo_{100-x} Alloys Grown on Cr Substrate

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We report the correlation between the magnetic properties and lattice parameter of Fe_xCo_{100-x} alloys as a function of constituent concentration. The saturation magnetization increases with Fe content and has a maximum value at approximately $x = 70$ at.%. However, collapse in relative saturation magnetization is observed at approximately 30 at.% to 70 at.% of Fe in Fe_xCo_{100-x} alloys. The collapse is due to the formation of Co-Co and Fe-Fe antibonding states instead of Fe-Co bonds. The lattice parameter also shrinks at approximately 30 at.% to 70 at.% of Fe. This shrinkage is due to an increase in the number of nearest neighbor antisite atoms, which then leads to a decrease in the long range order parameter.

Keywords : CoFe alloy, magnetic moment, lattice parameter

1. Introduction

Intermetallic compounds with a B2 structure show promise in high-temperature material applications due to their excellent physical and mechanical properties. B2-type intermetallic compounds are formed around the equiatomic composition in many binary alloys. Antisite atoms are intrinsically generated in these compounds through deviation of the composition from the stoichiometry, and strongly affect the physical and mechanical properties.

Particularly, Co and Fe alloys have attracted considerable attention in various technological applications because of their high Curie temperature, low magnetic anisotropy, and high saturation magnetization. Many experimental and theoretical studies have been carried out to investigate the composition dependent atomic structure and magnetic properties of Fe_xCo_{100-x} alloys. The Fe_xCo_{100-x} alloys form an ordered B2-phase (BCC) over a wide range of compositions. The Fe-Co phase diagram shows the presence of a BCC phase up to a Co content of 70 at.% [1]. The B2-phase alloys show ferromagnetism and transform to a disordered A2 structure at high temperatures with a wide concentration range at approximately 50 at.% Co. At around 1000 °C, the A2-phase transforms to an A1-phase, and the magnetic properties change from ferromagnetism to paramagnetism [2]. A two-phase (A1+A2) mixed region follows the B2-phase, and a single phase FCC region is then observed at 85-95 at.% Co. Experimental and theoretical studies have been carried out of the ferromagnetic properties of Fe_xCo_{100-x} alloys. The Slater-Pauling curve of the bulk magnetization of Fe_xCo_{100-x} alloys increases with Co concentration to a maximum at approximately 30 at.% Co and then decreases with further Co concentration [3].

Experimentally, BCC Fe_xCo_{100-x} alloy was first epitaxially grown on ZnSe/GaAs, the magnetization of which is tailored by varying the composition ratio [4]. This study was also significantly motivated by the surface induced unusual magnetic properties of spin reorientation transition on Cu (100) [5] and order-disorder magnetization on C (100) [6] with the Fe concentration of epitaxial grown ultra thin Fe_xCo_{100-x} alloy. In particular, it has been reported that molecular beam epitaxially (MBE) grown ultra thin film of Fe and Co forms a superlattice structure on the Cr interface layer [7, 8]. This report focuses on illustrating a nonmonotonic increase in the H_c and relative magnetic moment with Fe concentration on Fe_xCo_{100-x}/Cr (100).

In this paper, we present the results of the structural and magnetic properties of epitaxial FeCo alloys as a function of constituent concentration. The relative saturation magnetization and lattice parameter increase with Fe content;

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however, a collapse is observed in the relative saturation magnetization and shrinkage of the lattice parameter at approximately 30 at.% to 70 at.% of Fe in Fe_xCo_{100-x} alloys. This is due to an increase in the number of nearest neighbor antisite atoms.

2. Experimental Methods

The experiments were performed in an ultrahigh vacuum (UHV) system. The base pressure of the chamber was below 1.2×10^{-10} Torr. The Cr (100) substrate was cleaned using 1KV Ar ion sputtering and subsequently annealed at 900 K to produce a clear (1 × 1) surface structure. Fe_xCo_{100-x} alloys were deposited on the Cr (100) substrate at RT by co-evaporation of Co and Fe rods of 99.99% purity using the molecular beam epitaxial (MBE) method. The atomic ratio of Fe_xCo_{100-x} alloys were calculated using the comparable evaporation ratio of Fe and Co with a quartz-based thickness monitor. Magnetic properties were measured using the surface magneto optical Kerr effect (SMOKE) system and conducted on a UHV system with a He-Ne laser (632 nm wavelength). The linearly polarized incident beam was at about 45 degrees relative to the normal direction of the sample surface.

3. Results and Discussion

Figure 1 presents the thickness dependent H_c of $Fe_{50}Co_{50}$ alloys on the Cr (100) substrate. We considered thicknesses ranging from 1 monolayer (ML) to 10 ML. The hysteresis loops of the Co films were measured using the SMOKE technique with an in-situ electromagnet. Two different characteristics can be distinguished from the SMOKE measurement. Below 7 ML, the H_c increases with thickness, while above 7 ML the H_c decreases with thickness.

H_c is related to the rate of magnetic relaxation that occurs between the remanent and the demagnetized states. This relaxation process involves displacements of magnetic domain walls and the movement of magnetic domain walls can in turn be strongly affected by the thickness of the ferromagnetic layers [9]. It is known that the thickness dependence of H_c is closely correlated with the type of domain wall motion (i.e. Bloch or Néel); different types of domain wall motions would be expected to show different trends in the thickness dependence of H_c. It has been reported that the H_c is proportional to the film thickness for the Néel wall motion, but inversely proportional to the film thickness for the Bloch wall motion [10]. As shown in Figure 1, an increase in H_c has been clearly observed with increasing film thickness up to 7ML, indicating a Néel wall motion. While the film thickness increases further,

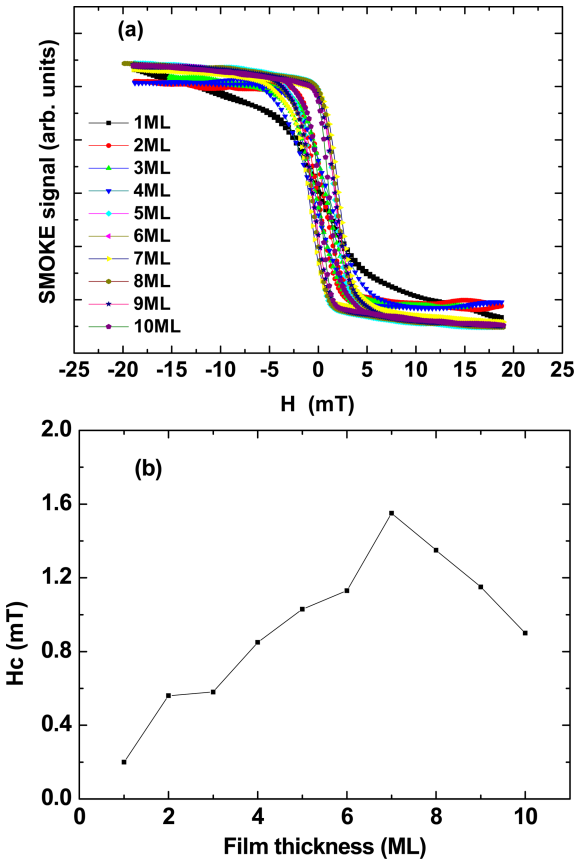

Fig. 1. (Color online) Thickness dependent H_c of $Fe_{50}Co_{50}$ alloys on Cr (100) substrate.

H_c decreases, suggesting a change in the type of domain wall motion from a Néel wall to a Bloch wall beyond 7 ML.

Figure 2 shows our experimental results of relative

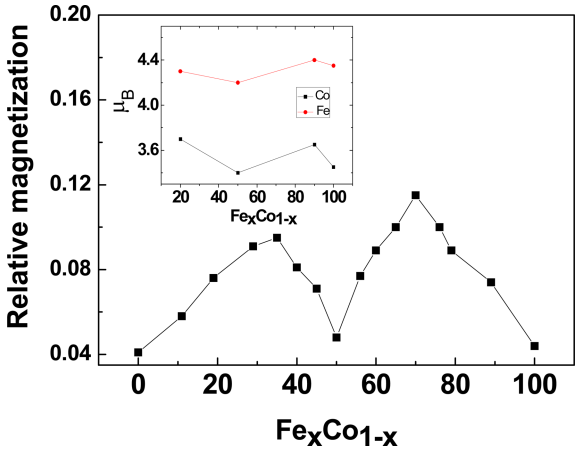

Fig. 2. (Color online) Relative saturation magnetization as a function of the Fe content in the Fe_xCo_{100-x} alloys. Theoretical results of partial magnetic moments are shown in the figure insert according to reference 11.

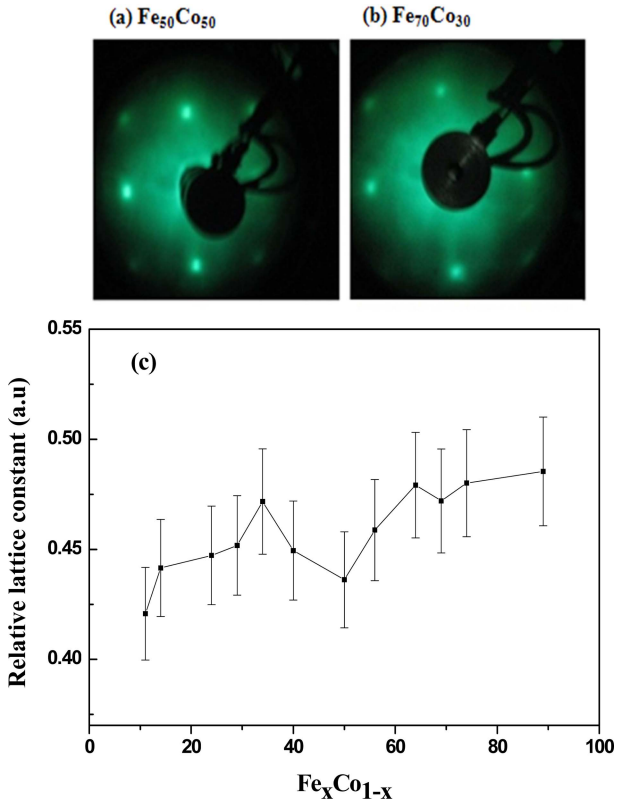

Fig. 3. (Color online) LEED patterns for (a) $Fe_{50}Co_{50}$ and (b) $Fe_{70}Co_{30}$, and (c) normalized lattice parameter with respect to the distance between two spots.

saturation magnetization as a function of the Fe content, x, in the Fe_xCo_{100-x} alloys, while the theoretical results of partial magnetic moments are shown as the figure insert [11]. The saturation magnetization increases with Fe content similar to the Slater-Pauling curve, where the saturation magnetization reaches a maximum value at approximately $x = 70$ at.%. Interestingly, the collapse in relative saturation magnetization is observed between 30 at.% and 70 at.% of Fe in Fe_xCo_{100-x} alloys.

The collapse in relative saturation magnetization near 50 at.% of Fe in Fe_xCo_{100-x} alloys is a result of the different electronic environments. The magnetic properties depend on the electronic structure because the d electrons are sensitive to local environment, and the presence of a dissimilar neighbor may thus cause an atom to exhibit a wide variety of behaviors. In an equiatomic FeCo alloy, Co atoms are located in a body-centered position and surrounded by Fe nearest neighbors, which are arranged at the corner position of a simple cubic lattice. Obviously, in FeCo alloys the magnetic moment is determined by the number of nearest neighbor atoms. Thus, the Fe moment increases with an increase in the number of nearest neighbor Co atoms. Moreover, this moment varies depending on whether the Fe atom concerned occupies Fe-site or Co-site. Theoretical results show that the nonmonotonic concentration dependence of the magnetic moment is caused by a change of the chemical composition of an alloy, which leads to a change of the partial contribution of the alloy's components to the magnetic moment [11]. Using the first-principle electronic-structure calculation for the defect and magnetic structure in Fe_xCo_{100-x} alloys, an antisite atom (Fe atom on the Co site and/or Co atom on the Fe site) can be formed in an off-stoichiometric composition [12]. Off-stoichiometric alloys in Fe-rich alloy (between 50% and 70 at.% Fe in Fe_xCo_{100-x} alloys) contain excess Fe atoms, while Co-rich alloy (between 30% and 50 at.% Fe in Fe_xCo_{100-x} alloys) contains excess Co atoms which results in the formation of an antisite atom. The antisite atoms should form antibonding states such as Co-Co bonds and Fe-Fe bonds instead of Fe-Co bonds, resulting in increments of antibonding states that are responsible for the decrease in magnetic moment.

Figure 3 shows the LEED patterns for (a) $Fe_{50}Co_{50}$ and (b) $Fe_{70}Co_{30}$, and shows (c) a normalized lattice parameter measured using the LEED image. The composition dependent lateral lattice parameters can be seen to increase linearly with increasing Fe content because the atomic radius of Fe is larger than that of Co. Similar to the relative saturation magnetization results, as shown in Fig. 2, the lateral lattice parameter also shrinks at approximately 30 at.% to 70 at.% of Fe in Fe_xCo_{100-x} alloys. As mentioned previously, an antisite atom can be formed in an off-stoichiometric composition. The long range order parameter (S) can be defined as [13]:

$$S = r_{Co} - y_{Co} = r_{Fe} - y_{Fe}$$

where r_{Co} and y_{Co} represent the concentrations of right Co atom and antisite Co atom, respectively, and similarly for r_{Fe} and y_{Fe}. Moreover, the lattice parameter (a) and magnetic moment (μ) are well approximated by a square of S:

$$a \propto S^2, \mu \propto S^2$$

Therefore, an increase in the number of nearest neighbor antisite atoms leads to a decrease in the S and results in a decrease in lattice parameter and magnetic moment.

4. Conclusion

We present the results of the structural and magnetic properties of epitaxial Fe_xCo_{100-x} alloys as a function of constituent concentration. The collapse of relative saturation magnetization observed in 30 at.% to 70 at.% of Fe in Fe_xCo_{100-x} alloys results from the formation of Co-Co and Fe-Fe antibonding states. The increment of the number

of nearest neighbor antisite atoms leads to a decrease in the long range order parameter, resulting in decreasing the lattice parameter.

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