Epitaxial growth and magnetic properties of Fe nanowedge islands on Mo(110)

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Abstract

Fe films with a nominal thickness ≥ 2 Å grown on Mo(110) at $500 \leq T \leq 750$ K self-assemble into nanowedge islands supported on a pseudomorphic Fe wetting layer. We propose a model explaining the island growth, which is based on the strain induced in the substrate around each island. Fe adatoms migrate towards the islands under the influence of this strain and subsequently enter the island through a vertical climb mechanism. We demonstrate that the magnetic properties of these nanostructures are governed by their shape. They do not display the in-plane spin reorientation transition found for the morphologically similar Fe/W(110) system.

Key words: self-assembly, iron, molybdenum, STM, SMOKE

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Scanning tunneling microscopy (STM) studies of the Fe/Mo(110) epitaxial system have shown that under elevated growth conditions, the Fe films self-assemble into nanowedge islands supported on a pseudomorphic wetting layer [1,2]. Similar results have been obtained by depositing Fe, Cu, Ni and Ho on W(110) [3,4,5,6] and Pb on Si(111) [7]. In this study, we explore the mechanisms guiding the nanowedge formation in the Fe/Mo(110) system and show how they are linked to the mismatch-induced strain. We have also investigated the magnetic properties of these nanostructures in-situ using surface magneto-optical Kerr effect (SMOKE) measurements.

The sample preparation and analysis were performed in ultra-high vacuum (UHV). Two Mo(110) substrates were used, with miscuts of 0.65° and 4.6° from the (110) plane, respectively. The first had an average terrace width of ~ 200 Å and monatomic steps aligned along the $[1\bar{1}\bar{1}]$ crystal direction. The second had an average terrace width of ~ 25 Å with monatomic steps oriented perpendicular to the $[1\bar{1}\bar{1}]$ direction. Each substrate was cleaned by annealing in 5×10^{-7} torr O_2 at $1300 \leq T \leq 1500$ K for 30-60 min cycles, followed by flash-annealing several times to 2400 K for 10-15 s in UHV. Fe films were deposited by e-beam evaporation of a 3N purity Fe rod at rates of 0.005 to 0.01 Å s^{-1} . The first Fe layer and up to 80 % of the second layer form nanowires on Mo(110) by the step-flow growth mechanism at 500 K [2]. The first Fe layer is a pseudomorphic wetting layer that is stable to 800 K [8]. However, dislocations are formed along the $[001]$ direction in second layer nanowires

above a critical wire width of ~ 100 Å [2]. Fe adatoms nucleate along these dislocations to form third layer protrusions as shown in Fig. 1a. When the protrusions on successive terraces overlap and coalesce, small nanowedges are formed (Fig. 1b). This is accompanied by a roughening of the step-edges as the second Fe layer breaks up and is absorbed into the nanowedges.

We propose that each nanowedge produces a localized strain in the substrate in its vicinity, which attracts adatoms to it. To illustrate this, we performed a finite element calculation on the simple model of a 1 nm thick Fe disk bonded to a Mo substrate. The diameter of the disk is in the range of 10 to 100 nm. The thickness and diameter of the substrate are 1000 nm and 2000 nm, respectively. The Fe disk is isotropically strained to reflect the 9 % lattice mismatch and in this expanded state it is bonded to the substrate. For the calculation we have used the stress-strain relation $\sigma = C(\epsilon - \epsilon_0)$, where ϵ_0 stands for the initial strain of the disk. The strain vector is given by

$$\begin{pmatrix} \epsilon_r \\ \epsilon_\theta \\ \epsilon_z \\ \gamma_{rz} \end{pmatrix} = \begin{pmatrix} \frac{\partial u}{\partial r} \\ \frac{u}{r} \\ \frac{\partial w}{\partial r} \\ \frac{\partial u}{\partial z} + \frac{\partial w}{\partial r} \end{pmatrix} \quad (1)$$

where r, z, θ are the coordinates of the cylindrical system, u and w are the radial and axial displacements respectively and are both independent of θ .

The tensor

$$C = \frac{E}{(1 + \nu)(1 - 2\nu)} \begin{pmatrix} 1 - \nu & \nu & \nu & 0 \\ \nu & 1 - \nu & \nu & 0 \\ \nu & \nu & 1 - \nu & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} \end{pmatrix} \quad (2)$$

includes the Youngs' modulus E and the Poisson's ratio ν for the isotropic material. Here we use E values of 211×10^9 (SI Units) and 329×10^9 (SI Units) and ν values of 0.33 and 0.293 for Fe and Mo, respectively. As the Fe disk relaxes inwards, it produces a tensile radial strain and compressive circumferential strain in the substrate surface outside its perimeter. Figure 2 shows the dependency of the radial strain component $\epsilon_r = \partial u / \partial r$ at the substrate surface as a function of the distance from the centre of disks of different sizes. As expected intuitively, islands of greater size create larger strained areas in the substrate.

The results of this simple model agree qualitatively with recent atomic scale calculations for Co islands on Cu(111), which have demonstrated that the Co islands induce an anisotropic strain in the substrate in their vicinity [9]. This strain influences the adatom diffusion in the vicinity of the island, since the adatom diffusion barrier shows a dependency on the surface strain. For compressive strain the diffusion barrier is reduced, for low tensile strain (≤ 4 %) it is increased and for large tensile strain it is reduced again [10]. In the Fe/Mo(110) system, the pseudomorphic Fe wetting layer accommodates a

large tensile strain (9 %), so that adatoms diffusing on this layer experience a low diffusion barrier. This barrier is lowered further in the vicinity of an island, which produces a radial pattern of increased tensile strain in the surrounding substrate. As a result, adatoms prefer to diffuse towards the island. As the size of the strained area depends on the island size, the adatom diffusion towards a nanowedge should be greater at its thicker end.

Upon reaching a nanowedge, the adatoms must undertake a vertical climb up each side of the island. We propose that dislocations in the lower layers of the nanowedge can act as diffusion channels to facilitate this vertical climb mechanism. The sites where dislocations thread to the walls of the island produce regions of compressive strain, which trap adatoms that diffuse along the edges of the island. The introduction of dislocations within the lower layers of the nanowedge also significantly reduces the lattice strain over these few layers. The lattice switches to the low tensile strain regime, where the adatom diffusion barrier decreases with decreasing tensile strain [10]. As a result, the further up the adatom climbs along the vertical wall of the island, the lower the diffusion barrier becomes. This results in anisotropic adatom diffusion towards the thick end of the nanowedge.

The longitudinal SMOKE measurements were performed in-vacuum at room temperature, on films grown on the vicinal Mo(110) surface. The films were deposited at room temperature and post-annealed at 750 K to form the nanowedge islands. Figure 3a shows an example of the islands grown on the vicinal sur-

face. The high step density produces an elongation of the islands along the direction of the step edges. It was found that for films grown at both 300 K and 750 K, the magnetic easy axis lay along the $[001]$ direction, neglecting the step-induced and shape anisotropy, while the hard axis lay along the $[1\bar{1}0]$ direction (Fig. 3b-e). Therefore, the Fe/Mo(110) system does not display the in-plane spin reorientation transition observed for the morphologically similar Fe/W(110) system [11]. Comparing Figs. 3d and e, it is clear that the nanowedge films display higher coercivity and saturation fields than their counterparts grown at 300 K. This is attributed to the demagnetising field associated with the shape of the nanowedges. The demagnetising field is higher for thicker nanowedges, which have a larger vertical aspect ratio (*c.f.* Figs. 3b and d). The elongation of the islands along the substrate step edges provides a shape anisotropy, which is superimposed on the magnetocrystalline anisotropy of the films. This slightly shifts the easy axis of magnetisation from the $[001]$ direction towards the step edge direction.

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Figure 1. $260 \text{ nm} \times 350 \text{ nm}$ STM images of a film with $3 \text{ \AA}$ nominal thickness grown on the low-index Mo(110) surface at $495 \pm 15 \text{ K}$. (a) Fe protrusions form along dislocations in the second Fe layer. (b) Protrusions on successive layers overlap and coalesce to form nanowedges. The second layer breaks up and is absorbed by these islands.

Figure 2. Calculated radial strain profile in a Mo substrate covered by 1 nm thick Fe disks of 5 , 25 and 50 nm radii, respectively. The tensile strain drops to 1% of its maximum value at approximately 9 , 18 and 22 nm from the edge of the 10 , 50 and 100 nm diameter disks, respectively.

Figure 3. (a) $200 \text{ nm} \times 200 \text{ nm}$ STM image of nanowedge islands grown on vicinal Mo(110) by depositing $4.5 \text{ \AA}$ Fe at 300 K and annealing to 750 K . (b), (c) Kerr loops taken along the $[001]$ and $[1\bar{1}0]$ directions, respectively, for a $6 \text{ \AA}$ film grown at 750 K . (d), (e) Easy axis Kerr loops taken for $10 \text{ \AA}$ Fe films grown at 300 K and 750 K , respectively.

Figure 1.

Figure 2.

Figure 3.