

## MAGNETIZATION ON VICINAL FERROMAGNETIC SURFACES

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### ABSTRACT

Using Ising model Monte Carlo simulations, we show a strong dependence of surface magnetization on surface miscut angle. For ferromagnetic surfaces, when surface spin exchange coupling is larger than that of the bulk, the surface magnetic ordering temperature decreases, toward the bulk Curie temperature, with increasing miscut angle; when surface spin exchange coupling is smaller than that of the bulk, a crossover behavior occurs: at low temperature, the surface magnetization decreases with increasing miscut angle; at high temperature, the reverse is true.

### INTRODUCTION

The magnetic properties of ferromagnetic surfaces and interfaces have been extensively investigated because of their potential impact on magnetic recording devices [1]. A large enhancement of magnetic moments at the surface of ferromagnetic materials is predicted by band structure theory [2-4]. The enhancement is attributed to the reduced dimension and coordination of surface atoms [2-4]. At ordinary temperatures, however, the fluctuations in the surface magnetization can be large enough to mask the possible differences in the magnetic moments of bulk and surface [5,6]. Although a direct measurement of surface magnetic moments remains a challenging problem, recent experiments have shown that the surface magnetization is different from that of the bulk. For example, in 4f rare-earth films, an enhanced surface magnetic ordering temperature has been observed [7-9], confirming the earlier theoretical predictions [10].

Most previous theoretical studies [2-5] of surface magnetism have been done on perfectly smooth surfaces assuming ideal bulk termination. However, in reality, surfaces contain variety of defects. The most abundant types of defects are steps which can arise, during the growth of a ferromagnetic film, from either a vicinal substrate or islands. Surface steps are expected to affect magnetism. For example, a recent experiment [11] shows that the dynamic response of a ferromagnetic surface (e.g., the shape of hysteresis curves) is dramatically altered by steps. In this article, we present a systematic theoretical study to establish the relationship of surface magnetization and its temperature dependence to surface miscut angle, i.e., step density. We find that surface steps strongly affect surface magnetization, not only changing the surface magnetic ordering temperature but also modifying the magnitude of magnetization in a complex fashion.

### SIMULATIONS

We simulate surface magnetization as a function of temperature for surfaces with different miscuts, using the Ising model Monte Carlo method. The simulations are performed on a simple cubic spin lattice slab with two free surfaces (see Fig. 1). Periodic boundary conditions are applied in the x- and y-directions. We use a basic sample size of 20×20×20 sites [12] and then add extra layers on the top surface to create different surface miscut angles, i.e., step

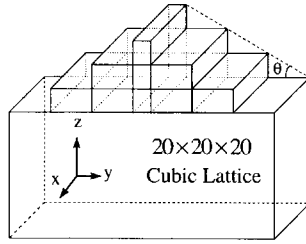


Figure 1. A schematic view of the spin lattices with a vicinal surface used in the Monte Carlo simulations.

densities. We use the nearest-neighbor Ising model to represent the interactions between the localized spins. The surface spin exchange coupling are chosen to be the same as or different from the bulk spin exchange coupling. We used 18,000 Monte Carlo steps in each simulation and the results are averaged over 5,000 steps after equilibration.

## RESULTS AND DISCUSSION

Figure 2 shows the surface magnetization as a function of temperature when the surface spin exchange coupling ( $J_s$ ) is set equal to the bulk spin exchange coupling ( $J_b$ ). The surface magnetization decreases with increasing miscut angle for all temperatures. This decreasing in magnetization with increasing miscut angle can be partly understood within the arguments of mean-field theory, in terms of modification of the effective local field of surface spins due to the surface steps. By assuming  $J_s = J_b$ , we treat the surface spins and bulk spins the same. The effective local field of a surface spin is simply proportional to its coordination number (see discussion below). In the vicinity of steps, the average coordination of surface spins decreases, and consequently, the surface magnetization decreases with increasing step density. Previous band structure calculations [4] also show that the magnetic moment of a ferromagnetic system displays a strong dependence on the local order of the atomic structure.

When  $J_s$  differs from  $J_b$ , the behavior of the surface magnetization with changing miscut angle is much more complex and intriguing.  $J_s$  may be larger or smaller than  $J_b$ . The reduced atomic coordination at a surface produces a narrower band width and hence a larger magnetic moment [2-4], favoring  $J_s > J_b$ . On the other hand, the surface lattice spacing can be larger than the bulk lattice spacing, leading to a weaker spin-spin interaction and favoring  $J_s < J_b$ . In 4f rare-earth films, e.g., Gd(0001), a surface magnetic ordering temperature higher than the bulk Curie temperature has been observed [9], indicating the system has  $J_s > J_b$  [13]. For 3d transition metals, indirect evidence from clusters points to the likelihood of  $J_s < J_b$  [6,14]. We therefore consider both possibilities.

Figure 3 shows an example of the dependence of magnetization on temperature for various miscuts of the vicinal surface for  $J_s > J_b$ . The surface magnetization always decreases with increasing surface step density, as for  $J_s = J_b$  (Fig. 2). For sufficiently high values of  $J_s$ , the surface magnetization can be higher than the bulk magnetization in the smooth surface but becomes smaller than the bulk magnetization as the miscut angle gets large. In agreement with previous simulations [13], we find that the surface has an ordering temperature above bulk Curie temperature ( $T_c$ ). Most importantly, however, we are able to show that the surface ordering temperature ( $T_{cs}$ ) decreases toward  $T_c$  as the surface miscut angle gets large. The

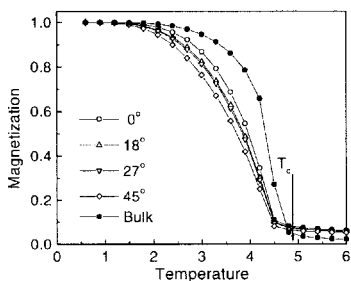


Figure 2. Surface magnetization as a function of temperature in vicinal surfaces with different miscuts, as shown in Figure 1, using  $J_s = J_b$ .  $T_c$  marks the bulk Curie temperature.

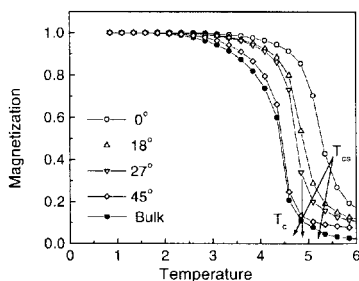


Figure 3. Same as Fig. 2, using  $J_s = 2J_b$ .  $T_{es}$  marks the surface ordering temperature.

enhancement of surface ordering temperature has been observed in Gd(0001) [9], and the enhancement is seen only in clean films. The disappearance of the enhancement on contaminated films is speculated to be due to surface roughness [9]. Our theory shows that surface steps can indeed lower surface ordering temperature without a need for impurities [15]. Experiments using clean samples with different degrees of surface miscuts, can confirm our prediction.

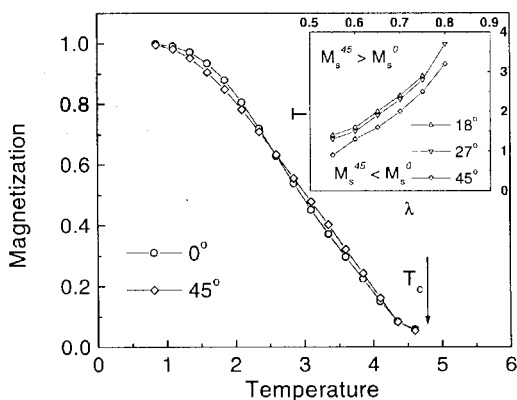


Figure 4. Surface magnetization as a function of temperature in vicinal surfaces, using  $J_s = 0.65J_b$  for a smooth surface and a  $45^\circ$  miscut surface. Notations are the same as in Fig. 2. The inset shows the dependence of the crossover temperature (relative to the smooth surface) as a function of the relative strength of  $J_s \propto \lambda^2$  for various values of miscut angles. The crossover temperature increases with increasing  $J_s$  and decreasing miscut angle.

A more complex behavior occurs when  $J_s < J_b$ . As an example, Figure 4 shows the dependence of the surface magnetization on temperature for  $J_s = 0.65 J_b$  in a smooth and a  $45^\circ$  miscut surface. Both surfaces start ordering at the bulk Curie temperature because the bulk ordering can induce the surface to order when  $J_s < J_b$ . The relationship of magnetization to miscut angle displays a crossover as a function of temperature. At low temperatures, the surface magnetization is higher in the smooth surface, while at higher temperatures, the surface magnetization is lower in the smooth surface. In Fig. 4, the crossover appears at about  $0.5T_c$ . In general, it depends on  $J_s$  and surface miscut angle. As shown in the inset of Fig. 4, for a given surface miscut angle, the crossover temperature increases monotonically with increasing  $J_s$ ; for a given  $J_s$ , the crossover temperature decreases with increasing miscut angle.

Although the crossover is not a phase transition, the inset of Fig. 4 resembles a phase diagram: in the upper left region, the surface magnetization increases with increasing surface miscut angle; in the lower right region, the surface magnetization decreases with increasing surface miscut angle. The fact that the crossover appears over a large range of values of  $J_s$  makes an experimental observation of this behavior plausible even though the differences in magnetization shown in Fig. 4 are not large.

## MEAN-FIELD THEORY

In order to understand the origin of the crossover behavior, we may apply mean-field theory to a vicinal surface. Within the nearest-neighbor Ising model, the effective local field of a surface spin,  $M_s$ , can be written as

$$M_s = z_s J_s m_s + z_b J_b m_b, \quad (1)$$

where  $z$ ,  $J$ , and  $m$  denotes respectively the number of nearest-neighbor spins, the exchange coupling, and the average magnetization. Subscripts  $s$  and  $b$  indicate surface and bulk, respectively. Assuming  $J_b = J$  and  $J_s = \lambda^2 J$ , the surface magnetization is derived as [16]

$$m_s = \tanh \left[ \frac{\lambda J}{k_B T} (\lambda z_s m_s + z_b m_b) \right], \quad (2)$$

where  $k_B$  is the Boltzmann constant. Now we compare two extreme surfaces: one with miscut angle  $0^\circ$ , perfectly smooth; one with miscut angle  $45^\circ$ , extremely rough. For the smooth surface,  $z_s = 4$  and  $z_b = 1$  in a simple cubic lattice. Equation (2) becomes

$$m_s^{smooth} = \tanh \left[ \frac{\lambda J}{k_B T} (4\lambda m_s + m_b) \right]. \quad (3)$$

For the  $45^\circ$  miscut surface,  $z_s = 2$  and  $z_b = 2$ . Equation (2) reduces to

$$m_s^{rough} = \tanh \left[ \frac{2\lambda J}{k_B T} (\lambda m_s + m_b) \right]. \quad (4)$$

For  $0.5 < \lambda < 1.0$ , it is easy to show that as  $T \rightarrow 0$ ,  $m_s, m_b \rightarrow 1$ . From eqns. (3) and (4) we have

$$m_s^{smooth} = 1 - 2 \exp\left[-\frac{\lambda J(4\lambda + 1)}{3k_B T}\right], \quad (5)$$

and

$$m_s^{rough} = 1 - 2 \exp\left[-\frac{2\lambda J(\lambda + 1)}{3k_B T}\right]. \quad (6)$$

As  $T \rightarrow T_c$  ( $T_c = 6J/k_B$  is the mean-field bulk Curie temperature),  $m_s, m_b \rightarrow 0$ ; then

$$m_s^{smooth} = \frac{\lambda m_b}{6 - 4\lambda^2}, \quad (7)$$

and

$$m_s^{rough} = \frac{\lambda m_b}{3 - \lambda^2}. \quad (8)$$

As a result,  $m_s^{smooth} > m_s^{rough}$  at low temperature but  $m_s^{smooth} < m_s^{rough}$  at high temperature, leading to the crossover behavior.

## CONCLUSIONS

We have investigated the behavior of surface magnetization on a vicinal surface. We show that the surface magnetic properties depend strongly on the surface miscut angle. Specifically, we establish that for surfaces with spin exchange coupling larger than the bulk, the surface magnetic ordering temperature is higher than the bulk Curie temperature and decreases toward bulk Curie temperature with increasing miscut. For surfaces with spin exchange coupling smaller than the bulk, a crossover behavior exists in the relationship of magnetization to miscut angle: the magnetization decreases at low temperature but increases at high temperature as the surface miscut angle increases. These predictions can be tested by experiments using vicinal surfaces with different miscuts.

## ACKNOWLEDGMENTS

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16. In deriving eqn. (2), the interaction between a surface spin and bulk spin is calculated as the geometric average of those between two surface spins and two bulk spins, as we did in the actual simulations. We have tested that the crossover will also appear at the extreme case when the interaction between a surface spin and a bulk spin is treated as equal to that between two bulk spins.