

## Noncollinear alignment of the surface and bulk magnetic moment in localized ferromagnets

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A model for noncollinear alignment between the surface-atomic-layer magnetic moment and bulk magnetic moment is proposed. It takes place due to the competition between ferromagnetic and antiferromagnetic exchange interactions of atomic layer with the nearest atomic layer and next-nearest atomic layer in the surface region. The criterion of the stability of surface state with collinear surface to bulk alignment is derived. On the basis of this criterion the phase diagram of surface magnetic states corresponding to a range of surface to bulk alignments at zero temperature is presented. We show that within this model the noncollinear surface to bulk alignment leads to a spiral magnetic structure in the surface region of a bulk ferromagnet. In the framework of this model a temperature-induced surface spin-reorientation transition takes place due to the change in the balance between exchange energies in the surface region with temperature. A self-consistent solution of the magnetization profile determination problem for any number of subsurface layers considered to be perturbed by the surface is used. In contrast to previous theoretical results we show that the increase in effective magnetic moment of a surface with temperature observed in experiments with Gd(0001), Tb(0001), and FeN<sub>3</sub> surfaces does not necessarily imply antiparallel alignment of surface and bulk magnetic moment at zero temperature. We demonstrate that this phenomenon is consistent with parallel surface to bulk alignment at low temperature as demonstrated in recent experiments on the Gd(0001) surface. [S0163-1829(97)01930-9]

### INTRODUCTION

Interest in noncollinear surface to bulk alignment in ferromagnets originates from the necessity for a physical treatment of the results of experiments that demonstrate both the enhancement of the surface Curie temperature with respect to the bulk Curie temperature and anomalous surface magnetic behavior near  $T_{Cb}$ . These phenomena are usually referred to as surface-enhanced magnetic order (SEMO) and surface magnetic reconstruction (SMR), respectively, and have been observed in experiments on Gd(0001) (Ref. 1) and Tb(0001) (Ref. 2) surfaces, as well as, the FeNi<sub>3</sub>(111), (Ref. 3) surface enriched by iron atoms. The authors of these experimental works made the proposition that the existence of a compensation point and increase in signal near the bulk Curie temperature ( $T_{Cb}$ ) is due to antiparallel of the topmost layer with respect to the bulk moment  $\mathbf{m}_b$ . Thus, the hypothesis of an antiparallel orientation of  $\mathbf{m}_1$  with respect to  $\mathbf{m}_b$  at  $T=0$  was formulated and subsequent *ab initio* calculations examined the structural, electronic, and magnetic properties of Gd(0001) taking into account the total system energy, indicating that the topmost Gd layer moment  $\mathbf{m}_1$  might be antiparallel with respect to the bulk magnetic moment.<sup>4</sup> These results are in direct contradiction with recent experiments on the Gd(0001) surface that conclusively demonstrated parallel alignment of the surface and bulk magnetic moment at low temperatures,<sup>5</sup> however, the description of the anomalous increase in signal was performed in the framework of spin models in the assumption of antiparallel surface to bulk alignment at  $T=0$ .<sup>6</sup> For this reason this problem is still unsolved. The observation of both SEMO and SMR phenomenon in markedly different systems, i.e.,

transition-metal alloys with itinerant electrons and rare earths with highly localized  $4f$  electrons, shows that this problem is rather general and interesting in itself.

Theoretical approaches to the description of increase in effective magnetic moment of the Gd(0001) surface<sup>7</sup> with temperature previously have been made in the framework of the following approximations: (1) Ising model, (2) the presence of nonzero external magnetic field, (3) a small number of layers (usually 3 or 4) considered to be perturbed by the surface, and (4) the assumption of antiparallel alignment of the surface and bulk magnetic moment in the bulk ferromagnetic (FM) material at zero temperature. It is very important to note that all four of these assumptions should not be made. The last assumption is clearly not valid in the light of recent experiments mentioned above. It is also well known that the bulk Gd magnetic moment lies in the basal plane at  $T=0$ . The increase in temperature leads to a spin reorientation of the bulk Gd moment to the  $c$  axis above 230 K, well below the bulk Curie point  $T_{Cb}=293.5$  K. The relatively small thickness of metal films used in experiments ( $<1000$  Å) together with the long-ranged magneto-dipole interaction force the vector moments to lie mainly in the surface plane. Therefore, an  $XY$  model for the description of magnetic properties of thin Gd films is more reasonable than the Ising model. In addition, it is essential that the original experimental measurements were performed in remanence, i.e., without the presence of an applied external magnetic field.<sup>1</sup> This means that an external magnetic field should not be considered as the physical reason for the surface magnetic moment behavior. Finally, the results of self-consistent calculations presented below show that for a particular set of parameters the temperature-induced spin-reorientation transition at the sur-

face requires one to account for up to ten or more atomic layers to be perturbed by the surface.

The deviation of the topmost atomic-layer moment  $\mathbf{m}_1$  orientation with respect to the direction of bulk moment  $\mathbf{m}_b$  of a ferromagnetic material is usually explained based on the difference between the surface and bulk anisotropy constants, taking into account the demagnetizing factor.<sup>8</sup> The mechanism of noncollinear ordering in the interface region due to roughness is also well known.<sup>9</sup> In the present paper a mechanism of noncollinear surface to bulk alignment for a FM material is proposed based on an  $XY$  model that includes the competition between the energies of exchange interaction of the topmost layer magnetic moment with the nearest- and next-nearest atomic layer moments. The first goal of the present article is the evaluation of the criterion of the stability of collinear surface to bulk alignment, independent of relative orientation, i.e., parallel or antiparallel. The second goal is the presentation of the phase diagram of various surface to bulk alignments. We also present a self-consistent model of the magnetization profile vs exchange interactions, and we investigate the evolution of surface magnetic states related to various kinds of surface to bulk alignment with temperature. This demonstrates that the competition of exchange interactions in the surface region gives rise to reorientation of atomic layer moments with temperature. The demonstration of temperature-induced spin-reorientation phase transitions in the surface region for two particular sets of model parameters is the third goal. We show that within this model the increase in the effective moment of a surface with temperature may be described in the assumption of parallel surface to bulk alignment at  $T=0$ , thus the experimental data on SMR available do not necessarily indicate nonparallel alignment of surface moment  $\mathbf{m}_1$  with respect to  $\mathbf{m}_b$  at  $T=0$ .

#### FORMULATION OF THE MODEL

Here we shall consider all the atomic layer vector moments  $\mathbf{m}_i$  to lie in the  $XY$  plane which is parallel to the surface plane of a film. The model we use for this work is an  $XY$  model with quasiclassical vector moments. This is applicable to these films because the Gd atom lies halfway through the rare-earth series with electronic configuration of  $[\text{Xe}]4f^75d^16s^2$ . In accordance with Hund's rule the half-filled  $f$  shell has the lowest energy for the maximum spin moment  $7\mu_B$ . Bulk atoms in Gd metal conserve this large moment due to (i) the large intra-atomic interaction in the  $4f$  shell, (ii) the absence of hybridization with conduction electrons, and (iii) the screening of  $f$  electrons by filled  $5s^25p^6$  shells. Therefore, from the point of view of the Gd band structure the conditions necessary for a spin Hamiltonian are satisfied. In addition, the wave functions of  $4f$  shells are highly localized, and the interaction between rigid  $f$  moments takes place due to Ruderman-Kittel-Kasuya-Yosida mechanism. This leads to an oscillatory dependence of exchange integrals on distance both in the bulk<sup>10</sup> and near the surface.<sup>11</sup> For this reason our consideration of phenomenological exchange integrals of different signs both in the bulk and in the surface region is natural. The validity of such a model was supported in recent calculations of spin configurations of  $\text{Gd}_{13}$  clusters.<sup>12</sup>

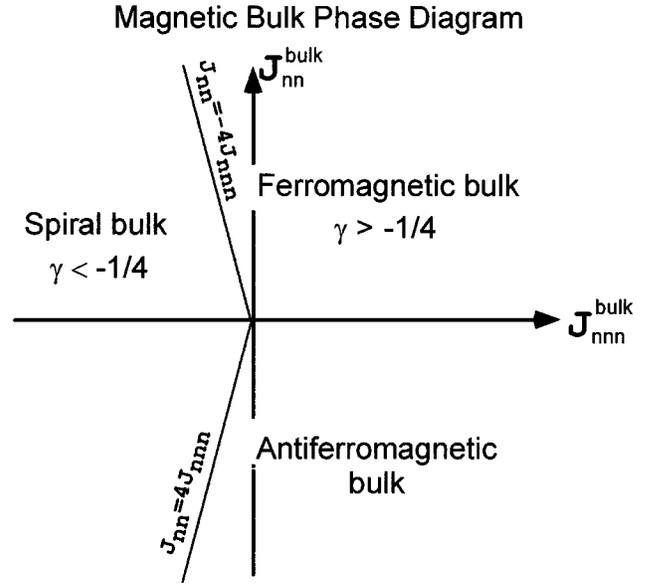


FIG. 1. The phase diagram of bulk magnetic states within an  $XY$  model for zero temperature in coordinates  $(J_{n,n+2}=L, J_{n,n+1}=J)$  with  $n$  is the layer index,  $n \gg 1$ . The bulk FM state is stable for  $J_{n,n+1}=J>0$  and  $-1/4 < \gamma = J_{n,n+2}/J_{n,n+1} = L/J$ .

The perturbation due to a surface can give rise to a change of exchange interactions that extends many atomic layers deep. For the present model, i.e., a magnetic slab of  $N$  layers, in principle all of the inter- and intralayer exchange interactions for  $n=1,2,3, \dots, N$  should be accounted for. However, a system with this many adjustable parameters is not justified for the description of the current experimental results. For this reason we consider the intralayer exchange interaction of a surface atom with its neighbors in the topmost atomic layer  $J_{11}$ , as the only one that differs from the similar exchange interactions in the rest atomic layers  $J_{nn}$   $n=2,3,4, \dots, N$ . Then we may denote  $\alpha J \equiv J_{11}$  and  $\delta J \equiv J_{nn}$  for  $n=2,3,4, \dots$ . Similarly, we write the interlayer exchange interaction in the bulk for an atomic moment with atoms in the next-nearest atomic layer  $\gamma J \equiv J_{n,n+2}$ . We consider the case of all the  $J_{n,n+2}$  equal to  $L \equiv \gamma J$  for every atomic layer throughout the whole crystal. Finally, we denote the first near-neighbor layer interaction as  $\beta J \equiv J_{12}$  and  $J \equiv J_{n,n+1}$  for  $n=2,3,4, \dots$ .

It is important to first investigate the bulk phase diagram to find the range of parameters where the ferromagnetic bulk state is stable. For this purpose one should consider the spiral state (SP) of the bulk where the moment rotates to some angle  $\varphi$  as one goes from one atomic layer to the next. In this case the atomic-layer magnetic moment  $\mathbf{S}_n$  can be written as  $\mathbf{S}_n = S(\cos\varphi n, \sin\varphi n)$ , where  $n$  is the atomic-layer index. The formula for the energy of a crystal with such a SP magnetic structure described above has the following form:

$$E = - \sum_n J(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) - \sum_n L(S_n^x S_{n+2}^x + S_n^y S_{n+2}^y) \\ \equiv S^2 \sum_n (J \cos\varphi + L \cos 2\varphi).$$

The minimization of this energy with respect to the angle  $\varphi$  gives rise to solutions  $\varphi=0$ ,  $\varphi=\pi$ , and  $\varphi=\arccos(-J/4L)$ .

These three solutions are the ferromagnetic (FM), antiferromagnetic (AF), and spiral (SP) cases, respectively, and the energies can be written as

$$E_{\text{FM}} = S^2 \sum_n (-J - L),$$

$$E_{\text{AF}} = S^2 \sum_n (+J - L),$$

$$E_{\text{SP}} = S^2 \sum_n \left( \frac{J^2}{8L} + L \right).$$

The direct comparison of energies  $E_{\text{FM}}$ ,  $E_{\text{AF}}$ , and  $E_{\text{SP}}$  with respect to each other allows one to construct the phase diagram for bulk magnetic states in coordinates  $(L, J)$ . This phase diagram is presented in Fig. 1. Below we restrict our consideration to the case of bulk FM state only. For this purpose we always will require the satisfaction of the following conditions:  $J \equiv J_{n,n+1} > 0$  and  $\gamma \equiv J_{n,n+2}/J_{n,n+1} \equiv L/J > -1/4$ .

### CRITERION OF NONCOLLINEAR SURFACE TO BULK ALIGNMENT

For the ferromagnetic bulk phase discussed above, the influence of the surface can be expected to cause the topmost atomic-layer moment to deviate from the direction of bulk magnetization. Here we consider an ideal surface that is uniformly magnetized in the plane of each layer. This reduces the problem to a semi-infinite one-dimensional  $XY$  model with the four adjustable parameters  $\alpha, \beta, \gamma, \delta$  defined above. Here we define the  $z$  axis to be perpendicular to the plane of the film, and  $\varphi_i$  is the angle between the  $i$ th atomic-layer moment  $\mathbf{m}_i$  and bulk magnetization vector  $\mathbf{m}_b$ . In accordance with the notation introduced above the spin-configuration energy has the following form:

$$\begin{aligned} E = & -\{ \beta J m_1 m_2 \cos(\varphi_1 - \varphi_2) + J m_2 m_3 \cos(\varphi_2 - \varphi_3) + \dots \\ & + \beta J m_{N-1} m_N \cos(\varphi_{N-1} - \varphi_N) + \gamma J [m_1 m_3 \cos(\varphi_1 - \varphi_3) \\ & + m_2 m_4 \cos(\varphi_2 - \varphi_4) + \dots \\ & + m_{N-2} m_N \cos(\varphi_{N-2} - \varphi_N)] \}. \end{aligned} \quad (1)$$

From this equation we proceed to evaluate the criterion for instability of the collinear (either parallel or antiparallel) surface to bulk moment alignment. Equation (1) can be rewritten in terms of the relative angles  $\alpha_i = \varphi_i - \varphi_{i+1}$ , i.e., the angles between neighboring atomic-layer vector moments  $\mathbf{m}_i$  and  $\mathbf{m}_{i+1}$ . Thus, we have  $N-1$  relative angles  $\alpha_i$  instead of  $N$  absolute angles  $\varphi_i$

$$\begin{aligned} E = & -JS^2 [ \beta \cos \alpha_1 + \cos \alpha_2 + \dots + \beta \cos \alpha_{N-1} \\ & + \gamma \cos(\alpha_1 + \alpha_2) + \gamma \cos(\alpha_2 + \alpha_3) + \dots \\ & + \gamma \cos(\alpha_{N-2} + \alpha_{N-1}) ], \end{aligned} \quad (2)$$

where for the two cases of collinear parallel and antiparallel surface to bulk alignment  $\alpha_1 = 0$  and  $\pi$ , respectively, and  $\alpha_2 = \alpha_3 = \dots = 0$ . Each angle  $\alpha_i$  is then varied away from the

corresponding collinear alignment and the perturbation on the energy is evaluated. For the case of small deviations  $\delta_i$  the expression for energy, Eq. (2), may be expanded to second order of every  $\delta_i$ :

$$E = E_0 + JS^2 \delta^T A \delta,$$

$$E_0 = -JS^2 [N - 3 \pm 2(\beta + \gamma) + (N-4)\gamma]. \quad (3)$$

The upper sign corresponds to the case of parallel surface to bulk alignment and the lower sign to the case of antiparallel alignment. For the sake of compactness we introduce vectors  $\delta = (\delta_1, \delta_2, \dots, \delta_{N-1})$  and  $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_{N-1})$ . In Eq. (3)  $A$  is a square  $(N-1) \times (N-1)$  three-diagonal symmetric matrix with real matrix elements for both parallel and antiparallel alignment, though  $A_{\uparrow\uparrow} \neq A_{\downarrow\downarrow}$  (see Appendixes A and B). The set of  $(N-1)$  eigenvectors  $\mathbf{a}_n$  of these matrices represents a full set of orthogonal vectors, i.e., it forms a basis in  $(N-1)$  dimensional space. Therefore, it is possible to expand vector  $\delta$  in eigenvectors  $\mathbf{a}_n$

$$\delta = c_1 \mathbf{a}_1 + c_2 \mathbf{a}_2 + \dots + c_{N-1} \mathbf{a}_{N-1}. \quad (4)$$

Then Eq. (3) may be rewritten in the following form:

$$E = E_0 + JS^2 \sum_{i=1}^{N-1} |c_i|^2 \Lambda_i. \quad (5)$$

Since we consider the case of the bulk ferromagnetic phase the exchange integral  $J$  should be considered positive (see Fig. 1). From Eq. (5) we find that for only positive sign of eigenvalues,  $\Lambda_i$ , the energy is minimal when every  $|c_i|^2 = 0$ . Using this condition in Eq. (4) shows that  $\delta = 0$ , i.e., the collinear (parallel or antiparallel) surface to bulk alignment is stable. On the other hand, if even one  $\Lambda_i$  becomes negative then the condition  $\delta = 0$  does not correspond to an energy minimum and collinear surface to bulk alignment becomes an unstable configuration. Thus, the criterion of instability of any collinear state of the surface is that the minimal eigenvalue of the corresponding matrix  $A$  should be less than zero.

This criterion allows one to obtain the condition of instability for any other collinear magnetic structure in the surface region. In addition, this criterion remains valid even in the case of an extended model that allows a greater number of layers to interact with a given layer.

### NONCOLLINEAR SURFACE TO BULK ALIGNMENT AT ZERO TEMPERATURE

On the basis of the criterion obtained above the conditions of instability of both parallel and antiparallel surface to bulk alignment may be expressed in terms of model parameters for the case of a semi-infinite crystal ( $N \rightarrow \infty$ ). The corresponding procedures are presented in Appendixes A and B, respectively. These conditions have the following form:

$$\text{if } \beta = \frac{J_{12}}{J} > \beta_F(\gamma) \equiv \frac{1 - \sqrt{1 + 4\gamma}}{2} \quad \text{and} \quad -1/4 < \gamma < +\infty,$$

$$\text{then } \mathbf{m}_1 \uparrow \uparrow \mathbf{m}_b; \quad (6.1)$$

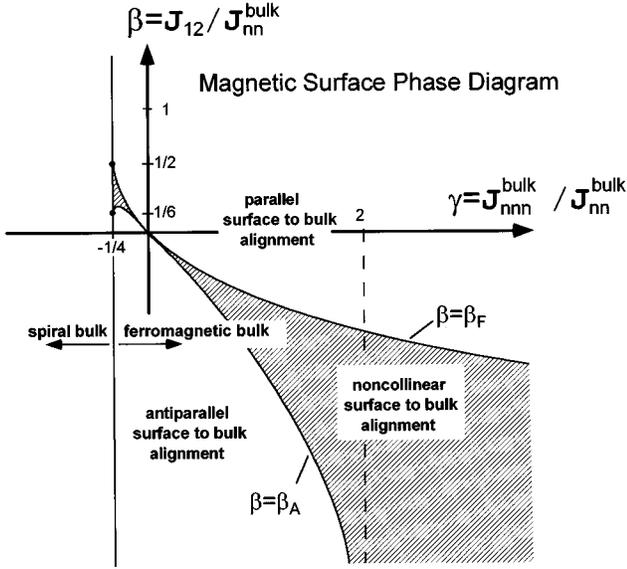


FIG. 2. The phase diagram of a surface magnetic states within the XY model for zero temperature in coordinates  $\beta = J_{12}/J$  and  $\gamma = J_{n,n+2}/J$ . The state with parallel surface to bulk alignment is unstable for  $\beta < \beta_F(\gamma)$ . The state with antiparallel surface to bulk alignment is unstable for  $\beta > \beta_A(\gamma)$  and  $-1/4 < \gamma < 2$ . If  $\gamma > 2$  then the state with antiparallel surface to bulk alignment is unstable for any value of  $\beta$ . A spiral magnetic structure exists in the surface region for  $\beta_A < \beta < \beta_F$  and  $-1/4 < \gamma < 2$ , and for  $\gamma > 2$  it takes place for any  $\beta < \beta_F$ .

$$\text{if } \beta = \frac{J_{12}}{J} < \beta_A(\gamma) \equiv \gamma \frac{3 + \sqrt{1+4\gamma}}{2(\gamma-2)} \text{ and } 0 < \gamma < 2, \quad \text{then } \mathbf{m}_1 \downarrow \uparrow \mathbf{m}_b; \quad (6.2)$$

if  $2 < \gamma < +\infty$ ,

then the state with  $\mathbf{m}_1 \downarrow \uparrow \mathbf{m}_b$  is never stable.

The plots of  $\beta_A(\gamma)$  and  $\beta_F(\gamma)$  defined in Eqs. (6.1) and (6.2) are presented in Fig. 2 and show regions corresponding to parallel and antiparallel surface to bulk alignment, respectively. These regions are separated by a finite interval for  $\gamma \neq 0$ . This interval corresponds to a noncollinear alignment of surface atomic layer moment with respect to the bulk. The existence of noncollinear surface to bulk alignment for the case  $\beta_A(\gamma) < \beta < \beta_F(\gamma)$  within the model proposed may be understood as a consequence of the balance between the energy of interaction of a surface moment  $\mathbf{m}_1$  with its nearest and next-nearest neighbors. For example, on the right-hand side of Fig. 2 we have  $\gamma = J_{1,3}/J > 0$ , i.e., the interaction between  $\mathbf{m}_1$  and  $\mathbf{m}_3$  favors parallel alignment between  $\mathbf{m}_1$  and  $\mathbf{m}_b$ . If  $\beta = J_{12}/J$  is also positive then it further stabilizes this configuration, however, if  $J_{12}$  is negative and of sufficient strength it can overcome  $J_{1,3}$ . The transitional state shown in Fig. 2 is only possible within an XY model where the spins are allowed to rotate freely in the surface plane, and the borders of this interval are given by the condition  $\beta_A(\gamma) < \beta < \beta_F(\gamma)$ .

In order to calculate the actual magnetization profile for the case  $\beta_A(\gamma) < \beta < \beta_F(\gamma)$  it is necessary to solve an infi-

nite set of equations after the minimization of energy, Eq. (2), with respect to every angle  $\alpha_1$

$$\begin{aligned} \beta \sin \alpha_1 + \gamma \sin(\alpha_1 + \alpha_2) &= 0, \\ \sin \alpha_2 + \gamma[\sin(\alpha_1 + \alpha_2) + \sin(\alpha_2 + \alpha_3)] &= 0, \\ \sin \alpha_3 + \gamma[\sin(\alpha_2 + \alpha_3) + \sin(\alpha_3 + \alpha_4)] &= 0, \\ &\vdots \\ \sin \alpha_n + \gamma[\sin(\alpha_{n-1} + \alpha_n) + \sin(\alpha_n + \alpha_{n+1})] &= 0. \end{aligned} \quad (7)$$

In the present paper we obtain the magnetization profile by means of iterative process originally developed by Camley.<sup>13</sup> It is based on the consequence of mean-field theory that the orientation of  $i$ th layer moment vector  $\mathbf{m}_i$  coincides with the direction of molecular field  $\mathbf{B}_i$  created by the neighboring atomic layer vector moments. The iterative process starts from the random initial spin configuration chosen for the first  $N_S \approx 10$  atomic layers and consists of successive correction of each vector moment  $\mathbf{m}_i$  along the direction of field vector  $\mathbf{B}_i$ . All other atomic layer spins ( $n = L+1, L+2, \dots$ ) are considered to be bulklike and are fixed in one direction. This iterative process gives a solution stable with respect to the initial profile, and the accuracy required. The number of atomic layers in the surface region considered to be perturbed by the surface  $N_S$  is increased until it does not lead to any change in the results obtained at the previous step. We find that the final state does not depend upon the initial spin configuration, showing the absence of any metastable states in the surface region, as expected for one-dimensional model.

The results of these calculations confirm the localization of borders  $\beta_A(\gamma)$  and  $\beta_F(\gamma)$  in the analytic phase diagram presented in Fig. 2. The noncollinear alignment of the topmost layer  $\mathbf{m}_1$  with respect to  $\mathbf{m}_b$  is observed and a spiral magnetic structure in the surface region is realized for  $\beta_A(\gamma) < \beta < \beta_F(\gamma)$ . The dependences of angles  $\varphi_i$  on the model parameter  $\beta = J_{12}/J$  for a given value of  $\gamma$  are presented in Fig. 3. This result is in accordance with the result of an analytical investigation of magnetization profile by means of corresponding differential equation on the function  $\varphi(i)$  obtained for asymptotic case  $i \gg 1$  from the last equation in Eq. (7);

$$\alpha_i = \varphi_i - \varphi_{i+1} \sim \exp\left[-i \frac{\sqrt{1+4\gamma}}{-\gamma}\right] \quad \text{for } \frac{-1}{4} < \gamma < 0, \quad (8.1)$$

$$\alpha_i = \varphi_i - \varphi_{i+1} \sim (-1)^i \exp\left[\frac{-i}{\gamma}\right] \quad \text{for } 0 < \gamma. \quad (8.2)$$

It is easy to see from Eqs. (8.1) and (8.2) that the profile depth depends only on the ratio of bulk exchange integrals  $\gamma = J_{n,n+2}/J$ . In particular, it follows from Eq. (8.1) that as  $\gamma$  approaches  $-1/4$ , i.e., as the point corresponding to the FM state of the bulk in Fig. 1 approaches the border with the SP state of the bulk, the depth of the SP profile approaches infinity. Thus, we see from both Fig. 3 and formulas (8.1) and (8.2) that the noncollinear surface to bulk moment alignment leads to a SP magnetic structure in the surface region.

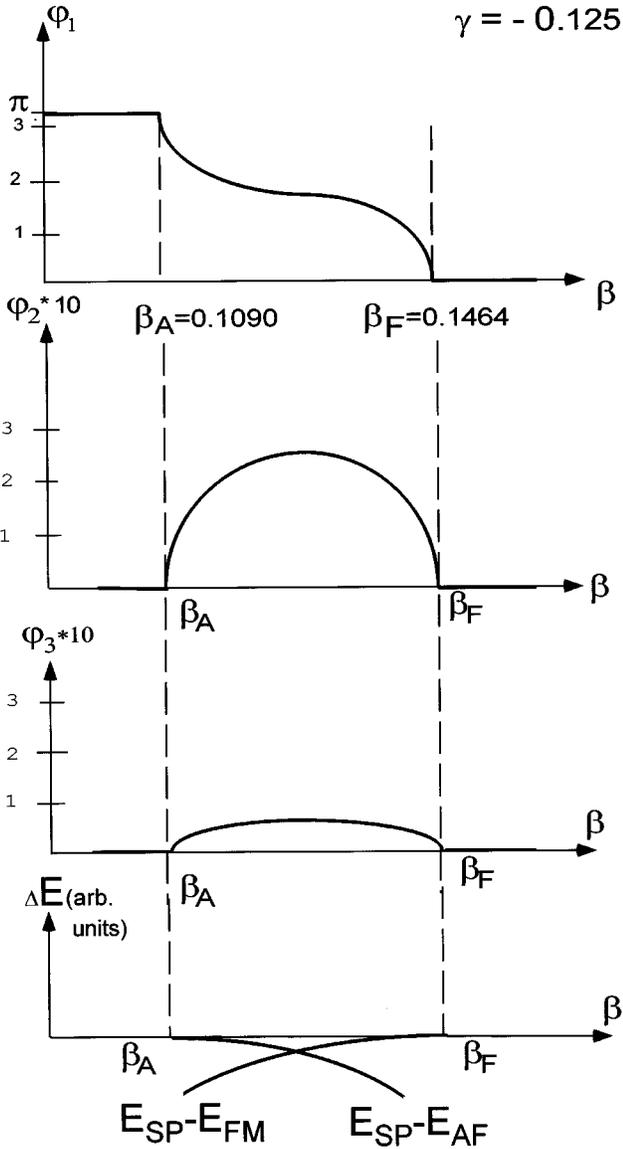


FIG. 3. The dependence of atomic layer moments orientation angles ( $\varphi_1, \varphi_2, \varphi_3$ ) on the interaction between the surface moment and the second layer moment  $\beta = J_{12}/J$  for  $\gamma = -0.125$  (top three panels). The dependence of energy differences  $\Delta E$  on  $\beta$  is shown in the bottom panel.  $E_{FM}$  is the energy of a crystal with parallel surface to bulk alignment,  $E_{AF}$  is the energy of a crystal with antiparallel surface to bulk alignment,  $E_{SP}$  is the energy of a crystal with spiral magnetic structure in the surface region.

#### TEMPERATURE-INDUCED SURFACE SPIN-REORIENTATION PHASE TRANSITIONS

For finite temperatures both the direction and thermally averaged magnitude of the magnetic moment of the atom in the  $i$ th layer must be specified. In order to calculate the temperature dependence of the surface magnetization the iteration process operates as follows. We first choose an arbitrary initial spin configuration in the first  $N_S$  ( $N_S \approx 10$ ) atomic layers with all the spins equal to  $S = 7/2$ . All other atomic-layer spins ( $n = N_S + 1, N_S + 2, \dots$ ) are considered to be bulklike and are fixed in one direction. The thermally averaged magnitude of spins in these bulk layers is obtained from the transcendental equation

$$\langle m_b \rangle = B_S \left( \frac{m_b H_b}{k_B T} \right),$$

where  $k_B$  is the Boltzmann constant,  $B_S(x)$  is the Brillouin function defined by the formula

$$B_S(x) = \left( S + \frac{1}{2} \right) \text{cth} \left[ x \left( S + \frac{1}{2} \right) \right] - \frac{1}{2} \text{cth} \left( x \frac{1}{2} \right),$$

and  $H_b$  is a molecular field that affects every atomic spin in the bulk,

$$H_b = (2\gamma + 2 + \delta) J m_b.$$

Thus, we know both the direction and the magnitude of all bulk spins for a given value of temperature  $T$ . We then allow the spin of an atom in the topmost layer ( $n = 1$ ) to rotate in the direction of the molecular field  $\mathbf{H}_{10}$  created by the neighboring spins in the second and the third atomic layers,

$$\mathbf{H}_{10} = \beta J \mathbf{m}_2 + \gamma J \mathbf{m}_3.$$

To obtain the thermally averaged magnitude of spin of an atom in the topmost atomic layer we solve the transcendental equation

$$\langle m_1 \rangle = B_S \left( \frac{m_1 H_1}{k_B T} \right),$$

where  $\mathbf{H}_1$  is the actual molecular field in the topmost layer. It differs from  $\mathbf{H}_{10}$  in that the contribution to molecular field from the neighbors in the topmost atomic layer is accounted for, i.e.,

$$\mathbf{H}_1 = \mathbf{H}_{10} + \alpha J \mathbf{m}_1.$$

The same procedure is done with spins of atoms up to the  $N_S$ th atomic layer. The corresponding molecular fields are defined by formulas

$$\mathbf{H}_{20} = \beta J \mathbf{m}_1 + J \mathbf{m}_3 + \gamma J \mathbf{m}_4, \quad \mathbf{H}_2 = \mathbf{H}_{20} + \delta J \mathbf{m}_2,$$

$$\mathbf{H}_{30} = \gamma J \mathbf{m}_1 + J \mathbf{m}_2 + J \mathbf{m}_4 + \gamma J \mathbf{m}_5, \quad \mathbf{H}_3 = \mathbf{H}_{30} + \delta J \mathbf{m}_3,$$

⋮

$$\mathbf{H}_{n0} = \gamma J \mathbf{m}_{n-2} + J \mathbf{m}_{n-1} + J \mathbf{m}_{n+1} + \gamma J \mathbf{m}_{n+2},$$

$$\mathbf{H}_n = \mathbf{H}_{n0} + \delta J \mathbf{m}_n,$$

⋮

$$\mathbf{H}_{L-1,0} = \gamma J \mathbf{m}_{L-3} + J \mathbf{m}_{L-2} + J \mathbf{m}_L + \gamma J \mathbf{m}_b,$$

$$\mathbf{H}_{L-1} = \mathbf{H}_{L-1,0} + \delta J \mathbf{m}_{L-1},$$

$$\mathbf{H}_{L,0} = \gamma J \mathbf{m}_{L-2} + J \mathbf{m}_{L-1} + J(1 + \gamma) \mathbf{m}_b,$$

$$\mathbf{H}_L = \mathbf{H}_{L,0} + \delta J \mathbf{m}_L.$$

The iterative process goes along this chain of  $N_S$  atomic layers until the accuracy required for a stable state is achieved ( $\Delta \varphi_i \approx 10^{-5}$ ,  $\Delta m_i \approx 10^{-3}$ ). This process is repeated

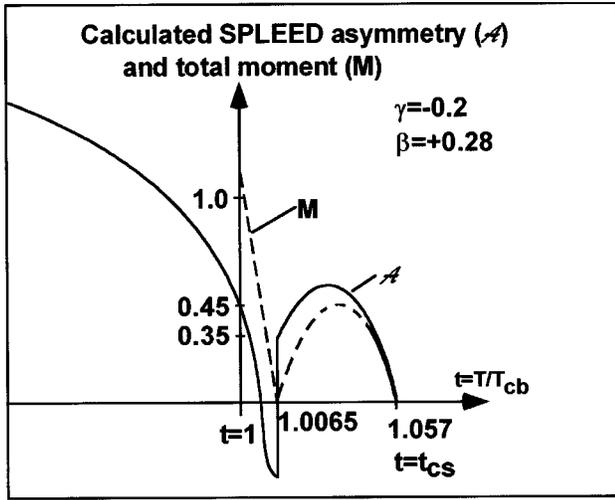


FIG. 4. The dependence of SPLEED asymmetry  $\mathcal{A}$  and total moment of a crystal  $M_{\text{tot}}$  on reduced temperature  $t=T/T_{cb}$  for  $\alpha=J_{11}/J=2.7$ ,  $\beta=J_{12}/J=0.3$ ,  $\gamma=J_{n,n+2}\equiv L/J=-0.2$ ,  $\delta=J_{n,n}/J=1$  ( $n=2,3,4,\dots$ ), and  $k=0.1$  for the case of parallel surface to bulk alignment at  $T=0$ .

for increasing numbers of subsurface atomic layers until there is no change in the results obtained relative to the previous step.

In order to compare our numerical results to the experimental spin polarized low energy electron diffraction (SPLEED) measurements it is necessary to calculate a weighted average of the surface magnetic region. We simulate the SPLEED asymmetry  $\mathcal{A}$  by using an exponentially decaying response function:

$$\mathcal{A} = \sum_{n=1}^{\infty} m_n \cos(\varphi_n) \exp(-\kappa n), \quad (9)$$

where  $\kappa \sim 10^{-1}$  for typical SPLEED energies.<sup>1</sup> The experimental results mentioned above also show that the surface has an enhanced Curie temperature  $T_{Cs}$ , with respect to bulk. We simulate this using an increased interlayer exchange coupling at the topmost layer. The analysis of the temperature dependence of the surface magnetization is rather complicated due to the large number of free parameters. In the present article, therefore, we consider only two points on the phase diagram,  $(\gamma, \beta) = (-0.2, +0.28)$  and  $(+0.5, -0.84)$ . These points are chosen to demonstrate how the SPLEED signal can be expected to behave with temperature for parallel and antiparallel  $T=0$  surface to bulk alignment, respectively.

For the first case,  $(\gamma, \beta) = (-0.2, +0.28)$ , i.e., parallel alignment of  $\mathbf{m}_1$  with respect to  $\mathbf{m}_b$  at  $T=0$ , we find that the parallel surface to bulk moment alignment is stable up to reduced temperature  $t_1 = T/T_{cb} = 0.450$ . Above this temperature, a continuous spin reorientation occurs as the topmost layer rotates in the  $X$ - $Y$  plane to the antiparallel orientation at  $t_2 = 0.879$ . Similarly, the second atomic moment undergoes a  $180^\circ$  continuous rotation from parallel to antiparallel between  $t_3 = 0.952$  and  $t_4 = 0.973$ . No other reorientations occurs for these particular values of  $\gamma, \beta$  up to  $t_{Cs}$ . The corresponding SPLEED asymmetry  $\mathcal{A}$  and the total moment  $M_{\text{tot}}$  of the entire sample are shown in Fig. 4. As expected  $\mathcal{A}$  goes negative before  $M_{\text{tot}}$  goes to zero because the

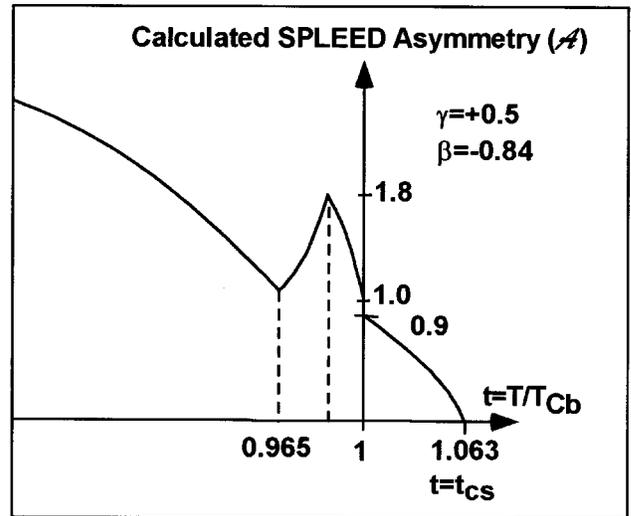


FIG. 5. The dependence of SPLEED asymmetry  $\mathcal{A}$  on temperature  $t=T/T_{cb}$  for  $\alpha=J_{11}/J=4$ ,  $\beta=J_{12}/J=-0.85$ ,  $\gamma=J_{n,n+2}\equiv L/J=0.5$ ,  $\delta=J_{n,n}/J=1$  ( $n=2,3,4,\dots$ ), and  $k=0.25$  for the case of antiparallel surface to bulk alignment at  $T=0$ .

SPLEED is sensitive to the first few atomic layers. Here, we show the signal going positive above the compensation temperature,  $t_0 = 1.0065$ , because the SPLEED measurements were made in remanence after applying a brief positive magnetizing pulse at every temperature. An important aspect of Fig. 4 is that both  $\mathcal{A}$  and  $M_{\text{tot}}$  continue to increase monotonically to their maximum value before going to zero at the surface Curie temperature,  $t_{Cs} = 1.057$ . This behavior corresponds closely to the actual experimental results,<sup>3</sup> and occurs within the present model due to the fact that the magnetization profile tail,  $m_3 + m_4 + m_5 + \dots$ , decreases with temperature more rapidly than magnetization of the first two layers,  $m_1 + m_2$ .

For the second case,  $(\gamma, \beta) = (0.5, -0.84)$ , i.e., antiparallel alignment of  $\mathbf{m}_1$  with respect to  $\mathbf{m}_b$  at  $T=0$ , we find a similar series of reorientation transitions with slight differences. For example, between  $t_1 = 0.965$  and  $t_2 = 0.975$  both  $\mathbf{m}_1$  and  $\mathbf{m}_2$  simultaneously rotate by  $180^\circ$ . This results in a spin configuration with only  $\mathbf{m}_2$  antiparallel to  $\mathbf{m}_b$ . In addition, we find that  $\mathbf{m}_4$  flips at  $t=1$ , resulting in a spin configuration with only  $\mathbf{m}_2$  and  $\mathbf{m}_4$  antiparallel to the bulk between  $t=t_{Cb}$  and  $t=t_{Cs}$ . This is due to the inclusion of an extended number of layers,  $N_S > 20$ , in the iterative process. The plot of  $\mathcal{A}$  vs  $t$  for this case is presented in Fig. 5. The increase in  $\mathcal{A}$  above  $t=0.965$  is due to the fact that  $m_1 > m_2$  in this temperature range. Above  $t_2 = 0.975$   $\mathcal{A}$  decreases as the magnetization goes to zero at  $t_{Cs}$ .

The plots of  $\mathcal{A}(t)$  shown in Figs. 4 and 5 resemble the experimental results from Gd(0001).<sup>1</sup> This shows that it is very difficult to distinguish these cases based on the available SPLEED data.<sup>1,3</sup> More recent spin-resolved secondary and photoemission electron spectroscopy show no sign change of the polarization above  $t_{Cb}$ .<sup>14</sup> In order to understand these results within our model it is necessary to investigate the temperature dependence of the surface for a wide range of parameters  $\alpha, \beta, \gamma, \delta$ . In addition, we are currently considering the contribution due to biquadratic exchange coupling and surface anisotropy. The results presented here

are an illustration of a more general concept, i.e., the consideration of the competing exchange integrals in the surface region of a localized spin system.

In conclusion, a model for the noncollinear surface to bulk alignment in a ferromagnet is proposed. In the framework of this model noncollinear alignment takes place due to the balance of competing exchange interactions in the surface atomic layer with the nearest and the next-nearest atomic layer. The criterion of noncollinear surface-bulk alignment was derived. On the basis of this criterion the phase diagram of the surface states corresponding to various coupling parameters is shown for zero temperature. The existence of a temperature-induced surface spin-reorientation transition is demonstrated for two particular sets of model parameters corresponding to parallel and antiparallel surface to bulk alignment at zero temperature. The increase in effective magnetic moment of a surface with temperature observed in experiments with Gd(0001), Tb(0001), and FeNi<sub>3</sub>, therefore does not necessarily indicate nonparallel alignment of surface moment with respect to bulk at low temperatures. This may be alternatively explained within the assumption of parallel surface to bulk alignment in correspondence with recent experimental data.

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#### APPENDIX A

Here we derive the analytic expression for the instability condition of a surface state with *parallel* surface to bulk

alignment in terms of model parameters. For this purpose we find the minimal eigenvalue of the matrix  $A_{\uparrow\uparrow}$  and require it to satisfy the criterion ( $\Lambda_{\min} < 0$ ) derived in the main text. The equation for eigenvalues  $\Lambda_i$  of the matrix  $A_{\uparrow\uparrow}$  corresponding to the case of parallel surface to bulk alignment is

$$\det A_{\uparrow\uparrow} = \det \begin{vmatrix} \varepsilon - k & 1/2 & 0 & 0 & 0 & 0 \\ 1/2 & \varepsilon & 1/2 & 0 & 0 & 0 \\ 0 & 1/2 & \varepsilon & 1/2 & 0 & 0 \\ 0 & 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon & 1/2 & 0 \\ 0 & 0 & 0 & 1/2 & \varepsilon & 1/2 \\ 0 & 0 & 0 & 0 & 1/2 & \varepsilon - k \end{vmatrix} = 0. \quad (\text{A1})$$

Here  $\varepsilon = \varepsilon_0 - \lambda$ ,  $\lambda = \Lambda/\gamma$ ,  $\varepsilon_0 = (2\gamma + 1)/(2\gamma)$ ,  $\kappa = (\gamma + 1 - \beta)/(2\gamma)$ . Thus, the parameter  $\kappa$  represents the surface perturbation caused by the absence of atomic layers above the surface. The analytic results following are obtained for the case of a semi-infinite crystal with a surface, i.e.,  $N \rightarrow \infty$ . This means that we may neglect the surface perturbation at the other surface of a film, i.e., we may set the parameter  $\kappa$  in the bottom right corner of the matrix  $A_{\uparrow\uparrow}$  to zero. Then Eq. (A1) may be rewritten as

$$d_{N-1} - k d_{N-2} = 0. \quad (\text{A2})$$

Here  $d_i$  is a determinant of a  $(i \times i)$  matrix similar to Eq. (A1) but with all the diagonal elements equal to  $\varepsilon$ , i.e., with  $\kappa = 0$ . For various values of  $\varepsilon$ ,  $d_i$  can be evaluated to find

$$d_i = \begin{cases} (-1)^i \frac{\sinh \varphi (i+1)}{2^i \sinh \varphi}, & \varepsilon < -1, \quad \varepsilon = -\cosh \varphi, \quad \varphi > 0, \\ \frac{\sin \varphi (i+1)}{2^i \sin \varphi}, & |\varepsilon| < 1, \quad \varepsilon = \cos \varphi, \quad \varphi > 0, \\ \frac{\sinh \varphi (i+1)}{2^i \sinh \varphi}, & \varepsilon > 1, \quad \varepsilon = \cosh \varphi, \quad \varphi > 0. \end{cases} \quad (\text{A3})$$

Since the expression for  $\varepsilon$  contains the eigenvalue  $\Lambda$  ( $\varepsilon = \varepsilon_0 - \lambda$ ,  $\lambda = \Lambda/\gamma$ ) the form of Eq. (A2) depends on the interval over which the eigenvalue axis is considered. This means that while searching for eigenvalues we should consider all the possible cases shown in Eq. (A3). Each separate case is shown below.

(1)  $|\varepsilon| < 1$ . In this case the reduced eigenvalues  $\lambda = \Lambda/\gamma$  belong to a ‘‘band’’

$$\varepsilon_0 - 1 < \Lambda/\gamma < \varepsilon_0 + 1.$$

(a) If  $\gamma > 0$  then the expression for the bottom of the corresponding band for eigenvalues  $\Lambda$  is equal to  $\gamma(\varepsilon_0 - 1)$ , and taking into account the expression for  $\varepsilon_0$  presented above, it is equal to  $1/2$ , i.e.,  $\Lambda > 0$ . Therefore, in this case there are no eigenvalues which could cross zero and become negative.

(b) If  $-1/4 < \gamma < 0$  (the left part of this double inequality means that the FM state of a bulk is still stable, as shown in Fig. 1) then the corresponding bottom of the ‘‘band’’ for  $\Lambda_i$  is when  $\Lambda = \gamma(\varepsilon_0 + 1) \equiv (4\gamma + 1)/2$ , i.e.,  $\Lambda_i > 0$ . The re-

sults of (a) and (b) show that eigenvalues which belong to a ‘‘band’’ can never cross zero, i.e., they are not able to satisfy the criterion derived.

We now consider the case of eigenvalues that are split from the ‘‘band’’.

(2)  $\varepsilon < -1$ . In this case Eq. (A2) may be written using Eq. (A3) in the form

$$2\kappa = \frac{d_{N-1}}{d_{N-2}} = -\frac{\sin\varphi N}{\sin\varphi(N-1)} \rightarrow -\exp(\varphi),$$

$$\varphi > 0, \quad N \rightarrow \infty. \quad (\text{A4})$$

Since  $\varphi > 0$  this equation has a solution for only the case  $2\kappa < -1$ . The corresponding eigenvalue which satisfies this equation is

$$\Lambda = \gamma[\varepsilon_0 + \cosh(\varphi)] = \gamma\left[\varepsilon_0 - \frac{1}{2}\left(2\kappa + \frac{1}{2\kappa}\right)\right]$$

$$= \frac{\gamma - (\beta^2 - \beta)}{2[\gamma - (\beta - 1)]}. \quad (\text{A5})$$

(3)  $\varepsilon > +1$ . In this case Eq. (A2) may be written using Eq. (A3) as

$$2\kappa = \frac{d_{N-1}}{d_{N-2}} = +\frac{\sin\varphi N}{\sin\varphi(N-1)} \rightarrow +\exp(\varphi),$$

$$\varphi > 0, \quad N \rightarrow \infty. \quad (\text{A6})$$

Since  $\varphi > 0$  this equation has a solution only for the case  $2\kappa > +1$ . The corresponding eigenvalue which satisfies this equation is

$$\Lambda = \gamma[\varepsilon_0 - \cosh(\varphi)] = \gamma\left[\varepsilon_0 - \frac{1}{2}\left(2\kappa + \frac{1}{2\kappa}\right)\right]$$

$$= \frac{\gamma - (\beta^2 - \beta)}{2[\gamma - (\beta - 1)]}. \quad (\text{A7})$$

Thus, we see that the expressions for  $\Lambda$  obtained for both  $\varepsilon < -1$  and  $\varepsilon > +1$  coincide. The solution of trivial inequality  $\Lambda < 0$  for the case  $\varepsilon < -1$ , i.e., for the case  $2\kappa < -1$  gives the result

$$\beta < \beta_F = \frac{1 - \sqrt{1 + 4\gamma}}{2} \quad \text{for } -1/4 < \gamma < 0. \quad (\text{A8})$$

The solution of the same inequality  $\Lambda < 0$  for the case  $\varepsilon > +1$ , i.e., for the case  $2\kappa > +1$  gives absolutely the same result for  $0 < \gamma < \infty$ . Thus, we have the same result (A8) in the entire interval of  $\gamma \in (-1/4, +\infty)$ , i.e., the condition of instability of the state of a surface with parallel surface to bulk alignment.

## APPENDIX B

Here we derive the analytical expression for the instability condition of a surface state with *antiparallel* surface to bulk magnetic moment alignment in terms of model parameters. In this case the equation on eigenvalues is

$$\det A_{\downarrow\uparrow} = \det \begin{vmatrix} \varepsilon - k & -1/2 & 0 & 0 & 0 & 0 & 0 \\ -1/2 & \varepsilon - 1 & 1/2 & 0 & 0 & 0 & 0 \\ 0 & 1/2 & \varepsilon & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 1/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/2 & \varepsilon - 1 & -1/2 \\ 0 & 0 & 0 & 0 & 0 & -1/2 & \varepsilon - k \end{vmatrix} = 0. \quad (\text{B1})$$

Here  $\varepsilon = \varepsilon_0 - \lambda$ ,  $\lambda = \Lambda/\gamma$ ,  $\varepsilon_0 = (2\gamma + 1)/(2\gamma)$ ,  $\kappa = (\beta + 3\gamma + 1)/(2\gamma)$ . Thus, we see that in contrast to the case of parallel surface to bulk alignment two matrix elements in both the upper left and the lower down corners of matrix  $A_{\downarrow\uparrow}$  differ from the corresponding matrix elements in the central part of the matrix [compare Eq. (B1) with Eq. (A1) in Appendix A]. This is due to the fact that the second atomic layer interacts with the antiparallel topmost layer. In other words, the surface perturbation extends for two atomic layers on each side of the  $N$  layer film. Below all the analytic results are obtained for the case of a semi-infinite crystal with a surface, i.e.,  $N \rightarrow \infty$ . Again we neglect the surface perturbation at the bottom of the film as in Appendix A. Then Eq. (B1) may be rewritten as

$$d_{N-1} - (\kappa + 1)d_{N-2} + \kappa d_{N-3} - 1/4 = 0. \quad (\text{B2})$$

Here  $d_i$  is a determinant of a  $(i \times i)$  matrix described in Appendix A and is determined by formula (A3). The expression for  $\varepsilon$  in Eq. (B1) contains the eigenvalue  $\Lambda$  that we are searching for ( $\varepsilon = \varepsilon_0 - \lambda$ ,  $\lambda = \Lambda/\gamma$ ). The form of the equation on eigenvalues depends on the interval on the eigenvalue axis considered, similar to the case of the parallel surface to bulk alignment. Therefore, we repeat the procedure described there, i.e., consider three possible cases.

(1)  $|\varepsilon| < 1$ . In this case the reduced eigenvalues  $\lambda = \Lambda/\gamma$  belong to a ‘‘band’’

$$\varepsilon_0 - 1 < \Lambda/\gamma < \varepsilon_0 + 1$$

and corresponding analyses gives the same result as the band case in Appendix A. As a result we have the same conclusion: all the eigenvalues which belong to a ‘‘band’’ can

never cross zero, i.e., they are not able to satisfy the criterion for instability of collinear alignment surface-bulk.

(2)  $\varepsilon < -1$ . In this case Eq. (B2) on eigenvalue  $\Lambda$  may be rewritten using Eq. (A3) in the form

$$\begin{aligned} & \sinh\varphi n + 2(\kappa + 1)\sinh\varphi(N-1) + 4\kappa \sinh\varphi(N-2) \\ & + 2 \sinh\varphi(N-3) = 0. \end{aligned} \quad (\text{B3})$$

Since  $\varphi > 0$  in the limit  $N$  approaches infinity we find

$$X^3 + 2(\kappa + 1)X^2 + 4\kappa X + 2 = 0, \quad (\text{B4})$$

where  $X = \exp(\varphi)$ . Since  $\varphi > 0$  we should only search for solutions  $X > 1$ . Analysis of the evolution of the roots of the latter equation depending on parameter  $\kappa$  shows the root  $X_0 > 1$  is possible in the case of  $\kappa < -5/6$  only. Further decrease in  $\kappa$  leads to an increase in  $X_0$ .

To determine when the eigenvalue corresponding to this root crosses zero, we obtain the condition for the following inequality:

$$\begin{aligned} \Lambda = \gamma\lambda = \gamma(\varepsilon_0 + \cosh\varphi) &= \gamma[(2\gamma + 1)/(2\gamma) + (X + X^{-1})/2] \\ &< 0. \end{aligned} \quad (\text{B5})$$

(a) In the case of  $\gamma > 0$  this inequality may be rewritten as

$$\frac{X^2 + 1}{2X} < -\frac{2\gamma + 1}{2\gamma}. \quad (\text{B6})$$

Since we may have only roots  $X > 1$  this inequality cannot be satisfied, and we have to consider the case of negative values of  $\gamma$ .

(b) In the case of  $-1/4 < \gamma < 0$  Eq. (B6) should be written in the following form:

$$\frac{X^2 + 1}{2X} > -\frac{2\gamma + 1}{2\gamma}. \quad (\text{B7})$$

Variation of  $\gamma$  in interval  $(-1/4, 0)$  allows one to satisfy the inequality (B7) with values of  $X$  that are greater than 1. In this range we find

$$X > -\frac{2\gamma + 1 + \sqrt{4\gamma + 1}}{2\gamma}. \quad (\text{B8})$$

The right side of this inequality is greater than 1 for  $-1/4 < \gamma < 0$ . Therefore, the investigation of Eq. (B4) on roots  $X > 1$  using inequality (B8) leads to the following conclusion: since inequality (B8) must be satisfied, the parameter  $\kappa$  in Eq. (B4) should be less than some critical value. This means that we must require the satisfaction of the following inequality:

$$2\kappa = \frac{\beta + 3\gamma + 1}{\gamma} < -\frac{X^3 + 2X^2 + 2}{X^2 + 2X}. \quad (\text{B9})$$

The solution of this inequality with respect to  $\beta$  using Eq. (B8) gives the following result for interval  $-1/4 < \gamma < 0$ :

$$\beta > \beta_A = \gamma \frac{3 + \sqrt{1 + 4\gamma}}{2(\gamma - 2)}. \quad (\text{B10})$$

(3)  $\varepsilon > +1$ . In this case a similar investigation leads to the same result (B10) for  $0 < \gamma < +2$ . However, if  $+2 < \gamma$  then the state with antiparallel alignment of surface to bulk moment is never stable.

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scopic in nature, and therefore the information depth is dependent on the electron energy. In the current article, for simplicity, we assume an experimental attenuation of the magnetization signal; see Eq. (9) with  $\kappa \sim 10^{-1}$ .

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