Magnetic properties of the semi-infinite Ising model with a surface amorphization

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Magnetic properties of the semi-infinite spin-$\frac{1}{2}$ Ising ferromagnet with a surface amorphization are investigated by the use of the effective-field theory with correlations. We find a number of characteristic behaviors for the surface magnetic properties, such as the possibility of surface reentrant phenomenon. The study of surfaces with amorphous layers may open a new field of surface magnetism.

I. INTRODUCTION

During the last decade, surface magnetism has received considerable interest both theoretically and experimentally. Experimentally, surface magnetic order has been studied mainly using crystalline systems such as Ni, Cr, and Gd.[1] Surface spin waves were also observed in an amorphous ferromagnetic alloy.[2] On theoretical grounds, many problems on the magnetism have been formulated by introducing simplified, yet not completely unrealistic models in which the surface plays an important role. Among them, the magnetic behavior of semi-infinite simple-cubic spin-$\frac{1}{2}$ Ising ferromagnet with the (100) free surface has received much attention and has been studied by using a variety of approximations and mathematical techniques, such as the mean-field approximation,[3] various effective-field theories,[4] series expansion,[5] Monte Carlo technique,[6] and renormalization-group method.[7] The standard example of surface magnetism includes two exchange interactions, represented by the bulk exchange parameter J and surface exchange parameter J_s. The system exhibits two successive transitions, namely, the surface and bulk phase transitions, as the temperature is lowered, and different types of phase transitions are associated with the surface. If the ratio $\Delta_s=(J_s/J)-1$ is greater than a critical value Δ_c, the system may order on the surface before it orders in the bulk. If the ratio is less than Δ_c, the system becomes ordered at the bulk transition temperature.

Surface treatment techniques using lasers to cover a wide surface with an amorphous layer has had growing success in recent years.[8,9] Laser glazing of a metallic alloy can be achieved by using a short laser pulse to melt a thin layer on the surface. Heat conduction into the bulk then gives a rapid quench rate and a thin amorphous surface layer is formed. From the technological point of view, the formation of an amorphous layer at a surface may be effective in improving the mechanical, magnetic, and corrosion resistance properties of a material with a free crystalline surface. Therefore, it is of great interest to investigate the magnetic properties of the semi-infinite simple-cubic Ising model with an amorphous magnetic layer. Even so, at this early stage, there is little in the literature concerning the magnetic problem.[10,11]

The purpose of this work is to study a semi-infinite simple-cubic spin-$\frac{1}{2}$ Ising ferromagnet with a disordered (100) surface (amorphized surface) by the use of effective-field theory with correlations.[12] The outline of this work is as follows: In Sec. II we present the basic points of the theory. In Sec. III we examine the phase diagram, which illustrates some interesting behaviors for the amorphizated surface, such as the possibility of a reentrant ferromagnetic surface phase. In Sec. IV the magnetization curves of surface are investigated numerically. We find a number of interesting phenomena for the thermal behavior of surface magnetization.

II. THEORY

We consider a semi-infinite simple-cubic spin-$\frac{1}{2}$ Ising model with an amorphous surface layer shown in Fig. 1. The Hamiltonian of the system is given by

$$\mathcal{H}=-\sum_{i,j} J_{ij}s_i^z s_j^z \ , \tag{1}$$

where s_i^z takes the values ± 1 and the summation is carried out only over nearest-neighbor pairs of spins. J_{ij} is the exchange interaction, which has the value $\bar{J}_s$ on the surface, the value $\bar{J}_1$ if one site is on the surface and its nearest-neighbor is at the next (first) layer. $\bar{J}_s$ and $\bar{J}_1$ are assumed to be randomly distributed according to the independent probability distribution functions $P(\bar{J}_s)$ and $P(\bar{J}_1)$.

The problem is now the evaluation of the mean value $\langle s_i^z \rangle$. Starting from an exact spin-correlation identity and using the differential-operator technique, we have developed the effective-field theory with correlations applied to the surface dilution problem,[12] which essentially corresponds to the Zernike approximation in the bulk problem.[13] The framework can be easily extended to the present problem. Following the formulation, for the surface magnetization σ_s, we obtain

$$\sigma_s=\langle\langle s_{i(=s)}^z\rangle\rangle_r=[\langle\cosh(D\bar{J}_s)\rangle_r+\sigma_s\langle\sinh(D\bar{J}_s)\rangle_r]^4[\langle\cosh(D\bar{J}_1)\rangle_r+\sigma_1\langle\sinh(D\bar{J}_1)\rangle_r]\tanh(\beta x)|_{x=0} \ , \tag{2}$$

where $\beta = 1/k_B T$ and $D = \partial/\partial x$ is a differential operator. The symbol $\langle \cdots \rangle_r$ denotes the random bond average. For the magnetization σ_1 of the first layer we have

$$\sigma_1 = \langle \langle s^z_{i(=1)} \rangle \rangle_r = [\cosh(DJ) + \sigma_1 \sinh(DJ)]^4 [\langle \cosh(D\bar{J}_1) \rangle_r + \sigma_s \langle \sinh(D\bar{J}_1) \rangle_r] \times [\cosh(DJ) + \sigma_2 \sinh(DJ)] \tanh(\beta x)|_{x=0} \, . \tag{3}$$

In general, the magnetization σ_n of the nth layer is given by

$$\sigma_n = [\cosh(DJ) + \sigma_n \sinh(DJ)]^4 [\cosh(DJ) + \sigma_{n-1} \sinh(DJ)][\cosh(DJ) + \sigma_{n+1} \sinh(DJ)] \tanh(\beta x)|_{x=0} \quad \text{for } n \geq 2 \, , \tag{4}$$

where σ_{n+1} and σ_{n-1} are the magnetizations in the $(n+1)$th and $(n-1)$th layers, respectively.

Now, in order to evaluate the random bond averages, it is necessary to provide the appropriate forms of the probability distribution functions $P(\bar{J}_s)$ and $P(\bar{J}_1)$, describing the structural disorder in a simple way. In a series of work[14] for the bulk amorphization we have used the probability distribution function $P(J_{ij})$ as

$$P(J_{ij}) = \tfrac{1}{2}[\delta(J_{ij} - J - \Delta J) + \delta(J_{ij} - J + \Delta J)]$$

with

$$\delta = \frac{\Delta J}{J} \, ,$$

where δ is a dimensionless parameter which measures the amount of fluctuation of exchange interaction. The parameter δ is often called as the structural fluctuation in amorphous magnets.[15] In this work, therefore, we take $P(\bar{J}_s)$ and $P(\bar{J}_1)$ as

$$P(\bar{J}_s) = \tfrac{1}{2}[\delta(\bar{J}_s - J_s - \Delta J_s) + \delta(\bar{J}_s - J_s + \Delta J_s)]$$

and

$$P(\bar{J}_1) = \tfrac{1}{2}[\delta(\bar{J}_1 - J_1 - \Delta J_1) + \delta(\bar{J}_1 - J_1 + \Delta J_1)] \, . \tag{5}$$

The random bond averages in Eqs. (2) and (3) are then given by

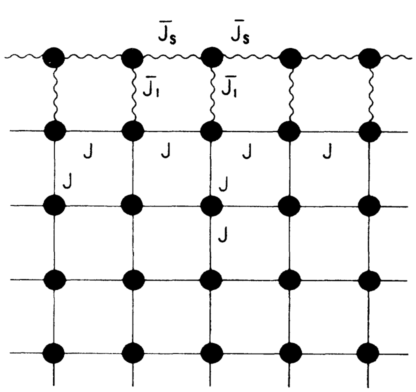

FIG. 1. Part of a two-dimensional cross section through the semi-infinite simple-cubic Ising lattice with an amorphous surface layer. Black points denote lattice points which are occupied by spins $s^z_i = \pm 1$. The straight lines indicate the bulk exchange interaction J, while wavy lines indicate exchange interactions J_s and J_1.

$$\langle \cosh(D\bar{J}_\alpha) \rangle_r = \cosh(DJ_\alpha \delta_\alpha) \cosh(DJ_\alpha) \, ,$$
$$\langle \sinh(D\bar{J}_\alpha) \rangle_r = \cosh(DJ_\alpha \delta_\alpha) \sinh(DJ_\alpha) \quad \text{for } \alpha = s \text{ or } 1 \, , \tag{6}$$

where we defined the parameter δ_α as

$$\delta_\alpha = \frac{\Delta J_\alpha}{J_\alpha} \quad \text{for } \alpha = s \text{ or } 1 \, . \tag{7}$$

The result (6) can also be obtained by using the so-called "lattice model" of amorphous magnets.[16]

III. PHASE DIAGRAMS

In this section we investigate the phase diagrams (or transition temperatures of surface and bulk) within the present formalism.

We are now interested in studying the transition temperature of the system. The usual argument that σ_i tends toward zero as the temperature approaches a critical temperature allows us to consider only terms linear in σ_i. Expanding the right-hand sides of (2), (3), and (4), we have

$$\sigma_s = 4K_1 \sigma_s + K_2 \sigma_1 \, , \tag{8}$$

$$\sigma_1 = 4K_3 \sigma_1 + K_4 \sigma_s + K_3 \sigma_2 \, , \tag{9}$$

and

$$\sigma_n = K(\sigma_{n-1} + 4\sigma_n + \sigma_{n+1}) \quad \text{for } n \geq 2 \tag{10}$$

with

$$\begin{aligned} K_1 &= \langle \sinh(D\bar{J}_s) \rangle_r [\langle \cosh(D\bar{J}_s) \rangle_r]^3 \times \langle \cosh(D\bar{J}_1) \rangle_r \tanh(\beta x)|_{x=0} \, , \\ K_2 &= \langle \sinh(D\bar{J}_1) \rangle_r [\langle \cosh(D\bar{J}_s) \rangle_r]^4 \times \tanh(\beta x)|_{x=0} \, , \\ K_3 &= \langle \cosh(D\bar{J}_1) \rangle_r \sinh(DJ) \cosh^4(DJ) \times \tanh(\beta x)|_{x=0} \, , \\ K_4 &= \langle \sinh(D\bar{J}_1) \rangle_r \cosh^5(DJ) \tanh(\beta x)|_{x=0} \, , \\ K &= \sinh(DJ) \cosh^5(DJ) \tanh(\beta x)|_{x=0} \, , \end{aligned} \tag{11}$$

where the coefficients (K_i and K) can easily be calculated by applying a mathematical relation $e^{\alpha D} f(x) = f(x + \alpha)$.

As discussed in Ref. 12, assuming that $\sigma_{n+1} = a\sigma_n$ for $n \geq 1$, Eqs. (8) and (9) yield the following secular equation:

$$\tilde{M}\begin{bmatrix}\sigma_s\\ \sigma_1\end{bmatrix}=\begin{bmatrix}4K_1-1 & K_2\\ K_4 & (4+a)K_3-1\end{bmatrix}\begin{bmatrix}\sigma_s\\ \sigma_1\end{bmatrix}=0\ . \quad (12)$$

The parameter a is given by, upon using (10),

$$a=\frac{(1-4K)-[(1-4K)^2-4K^2]^{1/2}}{2K}\ . \quad (13)$$

Thus, the critical ferromagnetic frontiers can be derived from the condition $\det\tilde{M}=0$, namely,

$$(4K_1-1)[(4+a)K_3-1]=K_2K_4\ . \quad (14)$$

From the formal solutions of (14) we choose those corresponding to the highest possible transition T_c^s which is the temperature for surface ordering. In our present treatment the bulk transition temperature T_c^b can be determined by setting $\sigma_n=\sigma_{n-1}=\sigma_{n+1}=\sigma_B$ into (10), namely, $6K=1$, which is equivalent to the Zernike equation obtained using another method.[13] The bulk transition temperature is then given by

$$\frac{k_B T_c^b}{J}=5.073\ .$$

This is an improvement on the traditional mean-field theory (MFT) (or $k_B T_c^{\mathrm{MFT}}/J=6$).

As noted in Ref. 17, it is important to remark here that when the transcendental function tanh$X$ appearing in the coefficients of our formalism are all replaced by their argument X, the critical frontiers obtained from (14), in general, reduce to those obtained within the framework of the standard MFT. In the present case, one can easily understand that the critical frontier becomes independent of δ_α ($\alpha=s$ or 1), when one applies the above argument to the coefficients, or when one uses the MFT and performs the random bond average in terms of (5). This is a shortcoming which is often seen in the usual MFT of amorphous ferromagnets when one uses the random distribution functions given by (5). As shown in the following, in our formalism the transition temperature is clearly dependent on surface structural fluctuations δ_α.

By solving Eqs. (13) and (14) numerically, we present some results on the phase diagram, introducing the following parameters:

$$J_s=J(1+\Delta_s),\quad J_1=J(1+\Delta_1)\ , \quad (15)$$

since the surface exchange interaction is often scaled with that of bulk in the statistical mechanics of surface magnetism.[3-7]

In Fig. 2 the results for $\delta_1=0$ are depicted in the Mills's sense. In Fig. 2 the curve labeled a with $J_1=J$ and $\delta_s=0$ expresses the surface-ordering critical line for a free crystalline surface. The critical value Δ_s^c for the surface ordering is given by $\Delta_s^c=0.3068$ ($\Delta_s^c=0.25$ for MFT[3]). As shown in Fig. 2 of previous work,[12] the results have been compared with those obtained from the standard MFT and high-temperature series-expansion methods. The critical value $\Delta_s^c=0.3068$ is also in excellent agreement with the renormalization-group result ($\Delta_s^c=0.307$).[18] On the other hand, the curve labeled a' is obtained for the system with $J_1=0.1J$ and $\delta_s=0$. Com-

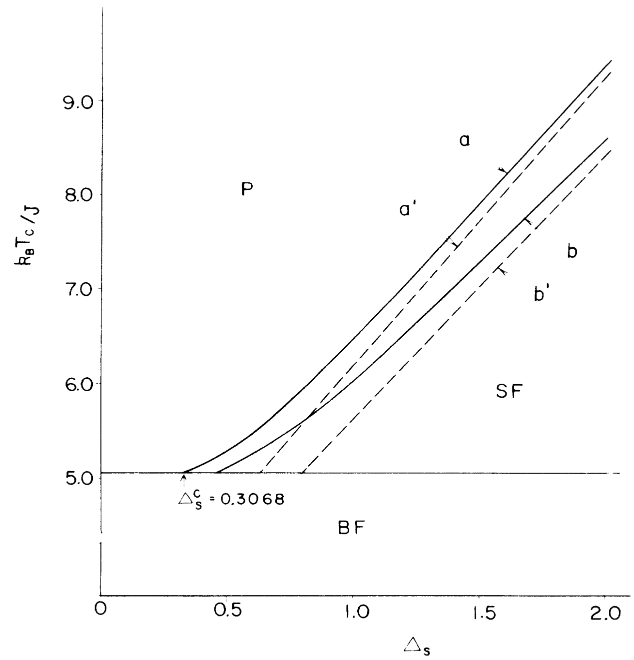

FIG. 2. The phase diagram in (T,Δ_s) space for the simple-cubic Ising model with a surface amorphization, when J_s is taken as $J_s=J(1+\Delta_s)$. Solid lines are obtained for $J_1=J$ and dashed lines are for $J_1=0.1J$. Curves a and a' are for the structural fluctuations ($\delta_s=\delta_1=0.0$). Curves b and b' are for $\delta_1=0.0$ and $\delta_s=0.5$.

paring with the two curves a and a', the behavior of T_c^s near the critical values of Δ_s is clearly different: curve a expresses a weak downward curvature of T_c^s whereas in curve a' T_c^s changes linearly with Δ_s. The difference does not change even when a weak surface amorphization ($\delta_s=0.5$) is included. The common effect of surface amorphization is to increase the critical value of Δ_s. In Fig. 2 we denote the paramagnetic, bulk-ferromagnetic, and surface-ferromagnetic phases by P, BF, and SF, respectively.

In Fig. 3 the surface ordering temperature T_c^s is plotted for three selected values of a pair (δ_s and δ_1), when J_s and J_1 are taken as $J_s=J$ and $J_1=J(1+\Delta_1)$. For curve a with a pure surface ($\delta_s=\delta_1=0$), the critical value of Δ_1 is given by $\Delta_1^c=0.550$, compared to the mean-field value $\Delta_1^c=1.0$. The effects of Δ_1 and δ_s on the SF phase are very similar to those of Fig. 2.

Now, it is known in an amorphous bulk ferromagnet that when the structural fluctuation δ becomes larger than the value of $\delta=1.0$, the reentrant phenomenon may appear, due to a random distribution in the sign of the exchange interaction.[15] Therefore, it is interesting to investigate whether the surface reentrant phenomenon is possible or not, when the surface structural fluctuation δ_s increases. In particular, the case of $\delta_s=1.0$ corresponds to the surface dilution problem with a concentration $P=0.5$. As is discussed in Refs. 12 and 19, the critical concentration P_c for the diluted system is given by $P_c=0.4248$ within the effective-field theory (EFT), so

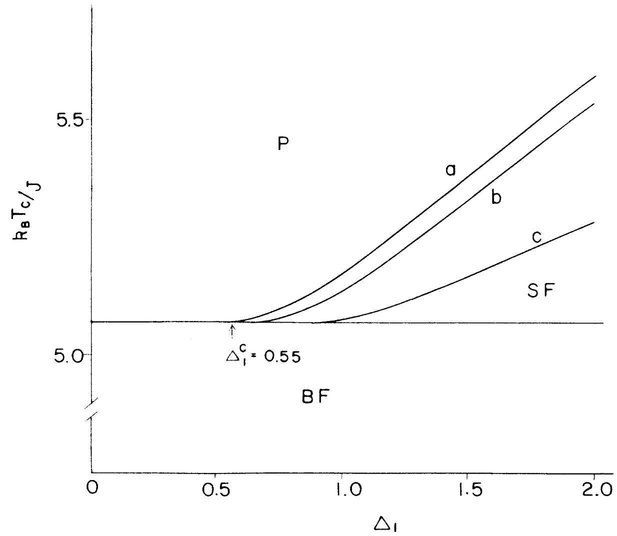

FIG. 3. The phase diagram in (T,Δ_1) space, when J_1 and J_s are taken as $J_1=J(1+\Delta_1)$ and $J_s=J$. Curves a, b, and c are obtained under the following conditions; (a) $\delta_s=\delta_1=0.0$, (b) $\delta_s=0.5$ and $\delta_1=0.0$, and (c) $\delta_s=\delta_1=0.5$.

that the surface is ferromagnetic even if $J_1=0$.[20] In Fig. 4 the surface ordering temperature T_c^s for a fixed value of J_s is plotted as a function of δ_s. The T_c^s for two values of J_1 ($J_1=J$ and $J_1=0.1J$) are also shown, in order to illustrate how the exchange interaction J_1 affects the SF phase. When the value of J_s is smaller than $J_s=2.0J$, as is shown by curve a, the value of T_c^s even for $J_1=J$ does not extend to the value of $\delta_s=1.0$, and hence, it is impossible to find the reentrant phenomenon on the surface. Moreover, for the curves b and c with $J_s=3J$ and $J_s=5J$, the surface reentrant phenomenon cannot be obtained, although for these parameters there is surface ordering at temperatures above T_c^b in the region of δ_s larger than $\delta_s=1.0$. For the (solid) curve d with $J_s=7J$ and $J_1=0.1J$, however, the surface reentrant phenomenon is observed in a very narrow region of δ_s, although the (dashed) curve d with $J_1=J$ does not exhibit such a phenomenon.

In Fig. 5 the change of T_c^s versus the values of δ_s larger than $\delta_s=1.0$ are depicted for the two values of J_s ($J_s=7J$ and $J_s=8J$), when J_1 is fixed as $J_1=0.1J$. The region of δ_s exhibiting the surface reentrant phenomenon becomes wider for $J_s=8J$ than for $J_s=7J$. Thus, we can conclude that the reentrant phenomenon is possible even on the surface, when J_s becomes larger than the bulk J and J_1 is taken as a value smaller than the bulk J.

IV. SURFACE MAGNETIZATION CURVES

In order to obtain the thermal behaviors of surface and layer magnetizations, it is necessary to solve the coupled equations (2), (3), and (4). For this purpose, we expand the right-hand sides of (2), (3), and (4), which gives

$$\sigma_s = 4K_1\sigma_s + K_2\sigma_1 + 4L_1(\sigma_s)^3 + 6L_2\sigma_1(\sigma_s)^2 + L_3\sigma_1(\sigma_s)^4 , \tag{16}$$

$$\sigma_1 = 4K_3\sigma_1 + K_4\sigma_s + K_3\sigma_2 + 4L_4(\sigma_1)^3 + 6L_5(\sigma_1)^2\sigma_s + L_6(\sigma_1)^4\sigma_s + 6L_7(\sigma_1)^2\sigma_2 + L_8(\sigma_1)^4\sigma_2 + 4L_5\sigma_1\sigma_2\sigma_s + 4L_6(\sigma_1)^3\sigma_2\sigma_s , \tag{17}$$

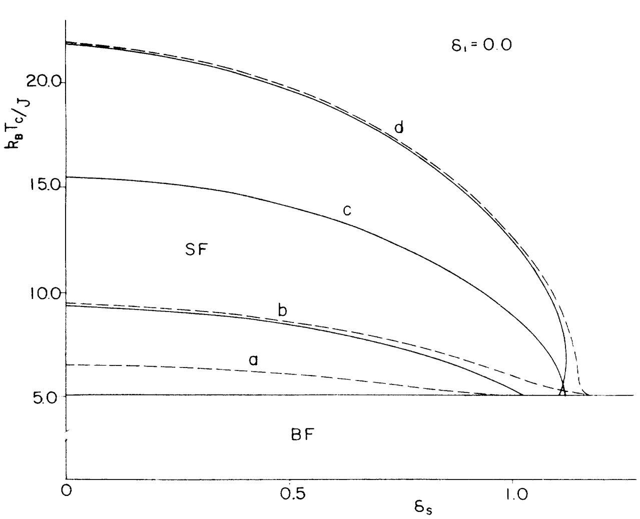

FIG. 4. The phase diagram in (T,δ_s) space for fixed values of J_s: curve a, $J_s=2J$; curve b, $J_s=3J$; curve c, $J_s=5J$; and curve d, $J_s=7J$. Two values of J_1 are then selected: solid lines are for $J_1=0.1J$ and dashed lines are for $J_1=J$.

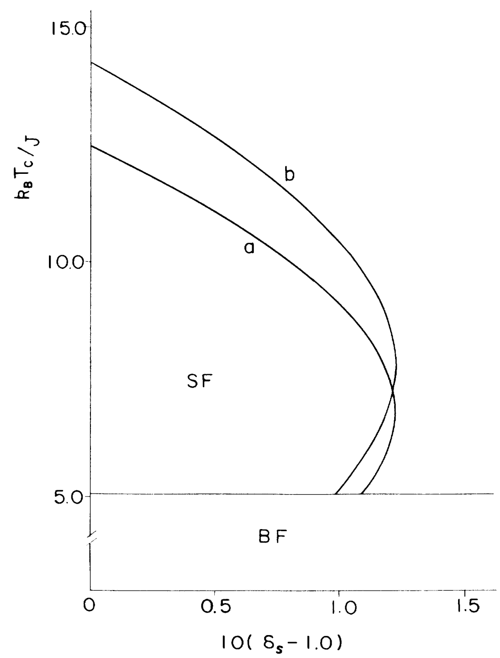

FIG. 5. The phase diagram in (T,δ_s) space for two values of J_s: curve a, $J_s=7J$ and curve b, $J_s=8J$. δ_1 and J_1 are fixed as $\delta_1=0.0$ and $J_1=0.1J$.

and

$$\sigma_n = (4\sigma_n + \sigma_{n-1} + \sigma_{n+1})K + [4(\sigma_n)^3 + 6\sigma_{n-1}(\sigma_n)^2 + 6\sigma_{n+1}(\sigma_n)^2 + 4\sigma_n\sigma_{n-1}\sigma_{n+1}]L$$
$$+ [\sigma_{n-1}(\sigma_n)^4 + \sigma_{n+1}(\sigma_n)^4 + 4(\sigma_n)^3\sigma_{n-1}\sigma_{n-1}]R \ , \qquad (18)$$

where the coefficients L_i ($i=1-8$), L, and R are given in the Appendix. On the other hand, as $n \to \infty$, σ_n should approach a bulk value σ_B determined from

$$\sigma_B = 6K\sigma_B + 20L(\sigma_B)^3 + 6R(\sigma_B)^5 \ . \qquad (19)$$

We are unable to solve the above coupled equations analytically. Even if we use a numerical method, they must be terminated at a certain layer. Therefore, the simplest method for solving them is to assume that the magnetization remains unaltered after the second layer, namely, $\sigma_2 = \sigma_3 = \cdots = \sigma_n = \sigma_B$, which may be called the three-layer approximation (as will be shown later, it is a rather powerful method for the evaluation of surface magnetization).

In the following, we show the numerical results based on the three-layer approximation. As shown in Sec. III, for $\Delta_s > \Delta_s^c$ the surface can behave, in the interval (T_c^b, T_c^s), like a bulk two-dimensional Ising system and for $\Delta_s < \Delta_s^c$ it orders when the bulk does.

In Fig. 6 the magnetization curves of surface as well as bulk are investigated for the system with $J_s = J$, $J_1 = J$, and $\delta_1 = 0$ (or the Mills model), changing the value of δ_s. The curve labeled a with $\delta_s = 0.0$ corresponds to the magnetization curve of a free crystalline surface. The magnetization curve changes linearly with T in the region of $4.0 < k_B T/J < 4.9$. Experimentally, such a linear temperature dependence of σ_s near $T = T_c^b$ has been observed in many semi-infinite crystalline magnets.[1]

As shown by the curves labeled b and c in Fig. 6, for the value of δ_s in the region $0 < \delta_s \le 1.0$, the surface magnetization shows a large depression from curve a (or the σ_s for the free crystalline surface) in the whole temperature range. In amorphous bulk ferromagnets such a depression of bulk magnetization from the corresponding crystalline has been generally observed.[15] In particular, the linear region of σ_s with T seems to become wider than that of $\delta_s = 0$ with the increase of δ_s, which is in contrast with the results of the MFT; when we apply the Handrich formula of amorphous bulk ferromagnets[16] to this problem, the linear region becomes narrower.[21]

On the other hand, when δ_s becomes larger than $\delta_s = 1.0$, the surface exchange interaction can take positive and negative values randomly; the so-called frustration due to the random distribution of J_s on the surface. Therefore, if we set $J_1 = 0$, the surface reduces to the two-dimensional bulk system (or square lattice), which can exhibit the reentrant phenomenon as well as the spin-glass phase, as discussed in Ref. 22. In Fig. 6, however, the surface is coupled to the first layer by the strong exchange interaction $J_1 = J$, so that the surface state behaves as if a strong magnetic field is applied to the two-dimensional frustrated bulk system. In fact, the curves labeled d, e, and f in Fig. 6 are very similar to those observed in Ref. 22. In particular, the increase of surface magnetization from the saturation value at $T=0$ K with the increase of T, as in curves e and f, comes from the release of frustrated spins due to the thermal disturbance.

Figure 7 shows the thermal behaviors of σ_s for the same system as that of Fig. 6 except that J_1 is taken as $J_1 = 0.1J$, changing the value of δ_s. Curve a corresponds to the surface magnetization with a free crystalline surface. The surface is coupled to the first layer by the weak exchange interaction $J_1 = 0.1J$, so that the surface mag-

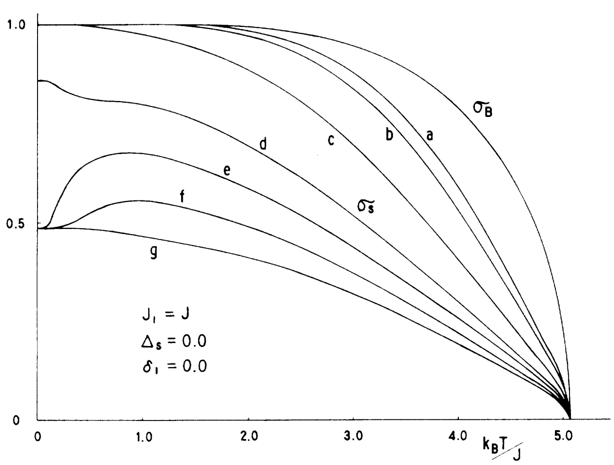

FIG. 6. Magnetization of surface and bulk for the system with $\Delta_s = \Delta_1 = 0.0$ and $\delta_1 = 0$, when the surface structural fluctuation δ_s is changed as follows: curve a, $\delta = 0.0$, curve b, $\delta_s = 0.5$; curve c, $\delta_s = 1.0$; curve d, $\delta_s = 1.4$; curve e, $\delta_s = 1.6$; curve f, $\delta_s = 1.8$; and curve g, $\delta_s = 2.0$.

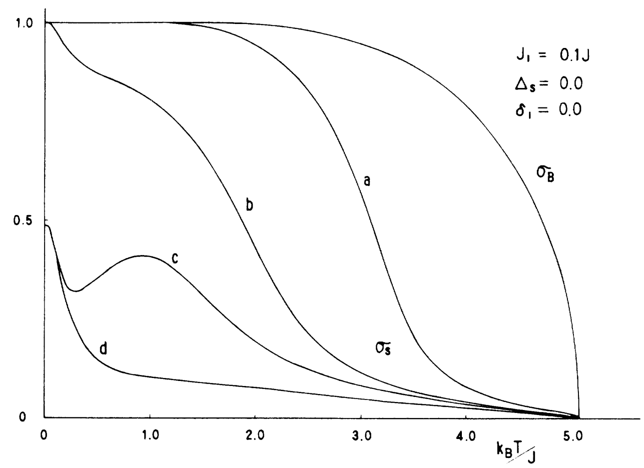

FIG. 7. The temperature dependence of σ_s for the system with $J_s = J$, $J_1 = 0.1J$, and $\delta_1 = 0.0$, when δ_s is changed as follows: curve a, $\delta_s = 0.0$; curve b, $\delta_s = 1.0$; curve c, $\delta_s = 1.2$; and curve d, $\delta_s = 1.6$. The magnetization curve of σ_B is also depicted.

netization (curve a) at first follows the two-dimensional bulk magnetization [the bulk transition temperature for $z=4$ is given by $k_B T_c^b(z=4)/J=3.090$, where z is the coordination number[19]], takes small values above $T=T_c^b(z=4)$, and reduces to zero at the bulk transition temperature $k_B T_c^b/J=5.073$.

In Fig. 7, we also observe characteristic behavior for σ_s, when δ_s becomes larger than $\delta_s=1.0$. In particular, the curve labeled c with $\delta_s=1.2$ exhibits a minimum and a maximum with increasing T, which corresponds to the trace of the reentrant phenomenon observed in the two-dimensional frustrated bulk ferromagnet. As mentioned above, the surface state just corresponds to that of the frustrated bulk system in a weakly applied field. In fact, such behavior is observed in Ref. 22, when a weak magnetic field is applied to the bulk system showing the reentrant phenomenon.

As discussed in Sec. III, $\Delta_s=0.3068$ just corresponds to the multicritical point for the Mills model (namely, $J_s=J$, $J_1=J$, and $\delta_s=\delta_1=0$) with a free crystalline surface (see Fig. 2). Both the surface magnetization as well as the first layer should be then equivalent to that of bulk.

In Fig. 8 surface magnetization (solid curves) is investigated for the system with $J_s=1.3068J$, $J_1=J$, and $\delta_1=0$, changing the value of δ_s. On the other hand, the three solid-dashed curves correspond to surface magnetization for the system with $J_s=1.3068J$, $J_1=J$, and $\delta_1=1.4$, when the value of δ_s is selected as $\delta_s=0.5$, $\delta_s=1.4$, and $\delta_s=1.8$. For $\delta_s=\delta_1=0$, as expected, the curve of σ_s in the Mills sense is equivalent to that of σ_B as well as σ_1 within the numerical errors. The solid curves a and b with $\delta_s=0.5$ and $\delta_s=1.0$ also express a rather large depression from that of $\delta_s=\delta_1=0.0$.

Characteristic behavior of σ_s, which could not be inferred only from the phase diagrams of Sec. III, is also observed when compared with the corresponding curves of Fig. 8; the surface magnetization represented by curves c and c' (or the curves d and d') have the same values for J_s, δ_s, and J_1, except that δ_1 takes two different values ($\delta_1=0$ and $\delta_1=1.4$). The corresponding curves change their shapes in the low-temperature region, where J_1 takes positive and negative values randomly, although curves a and a' do not.

When Δ_s becomes larger than the critical value Δ_s^c, the SF phase may appear above the bulk transition temperature, as shown in Sec. III. Figure 9 shows the thermal behavior of σ_s for the system with $J_s=3J$, $J_1=J$, and $\delta_1=0$ when δ_s is changed. As is understood from the dashed curve b of Fig. 4, when δ_s becomes larger than $\delta_s=1.16$, the SF phase disappears, so that the surface magnetization labeled by curve e with $\delta_s=1.2$ in Fig. 9 reduces to zero at $T=T_c^b$. For the value of δ_s in the region $0\le\delta_s\le 1.16$, on the other hand, the surface magnetization has finite values even for T larger than T_c^b, as predicted in Sec. III.

In Fig. 5 we have found the possibility of surface reentrant phenomenon, when J_s is taken as $J_s=8J$ (or $J_s=7J$) and J_1 is fixed at $J_1=0.1J$. In Fig. 10, therefore, the temperature dependence of σ_s is investigated for the system with $J_s=8J$, $\delta_s=1.1$, and $\delta_1=0$, selecting the two values of J_1 ($J_1=0.1J$ and $J_1=J$). The surface reentrant phenomenon is obtained for the case of $J_1=0.1J$ in the temperature region above $T=T_c^b$, although it does not appear for $J_1=J$, which is consistent with the results of Fig. 5.

In Fig. 10, the characteristic behavior of σ_s is also illustrated. The first is the discontinuity of the derivative of σ_s at $T=T_c^b$, obtained for the curve with $J_1=J$. Such a discontinuity has not been observed in the curves of Fig. 9. The second is the thermal behavior of δ_s for

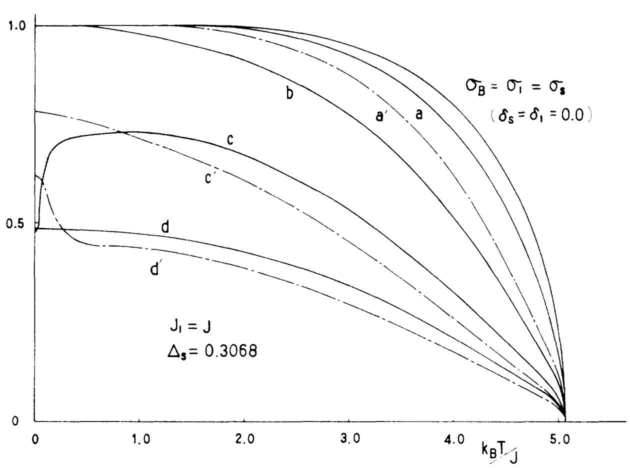

FIG. 8. Magnetization curves of surface for the system with $\Delta_s=0.3068$ and $\Delta_1=0.0$. Solid lines are obtained by fixing the value of δ_1 as $\delta_1=0.0$ and changing the value of δ_s as follows: $\delta_s=0.0$, curve a, $\delta_s=0.5$; curve b, $\delta_s=1.0$; curve c, $\delta_s=1.4$; and curve d, $\delta_s=1.8$. Solid-dashed lines are obtained by fixing the value of δ_1 as $\delta_1=1.4$ and changing the value of δ_s as follows: curve a', $\delta_s=0.5$; curve c', $\delta_s=1.4$; and curve d', $\delta_s=1.8$.

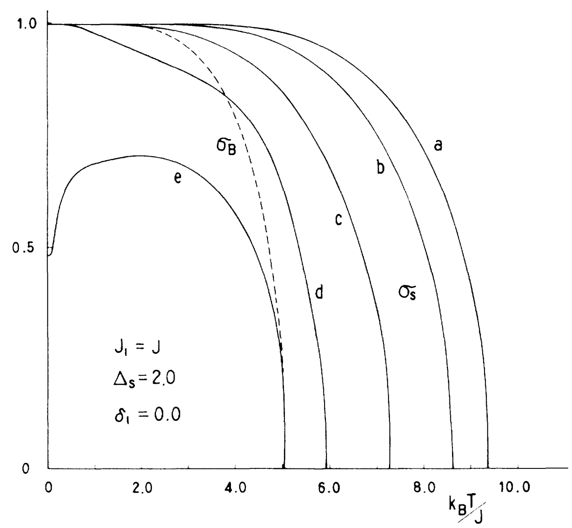

FIG. 9. The temperature dependences of σ_s for the system with $\Delta_s=2.0$, $\Delta_1=0.0$, and $\delta_1=0.0$, when δ_s is changed as follows: curve a, $\delta_s=0.0$; curve b, $\delta_s=0.5$; curve c, $\delta_s=0.8$; curve d, $\delta_s=1.0$; and curve e, $\delta_s=1.2$. The dashed line expresses the magnetization of σ_B.

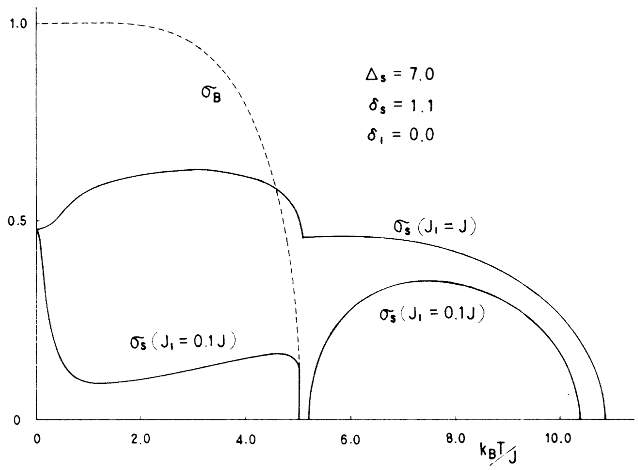

FIG. 10. Magnetization of surface for the system with $\Delta_s=7.0$, $\delta_s=1.1$, and $\delta_1=0.1$, when J_1 is selected as $J_1=J$ and $J_1=0.1J$. The dashed line expresses the bulk magnetization σ_B.

$J_1=0.1J$ in the temperature range below $T=T_c^b$; it has finite values and furthermore shows a minimum and maximum in the region of T studied. Such a phenomenon comes from the fact that frustrated spins on the surface are coupled to the ferromagnetic layers and are apt to align to the z direction in the temperature range, even if the surface reentrant phenomenon is observed above $T=T_c^b$.

In the above discussions, we have introduced the three-layer approximation in order to obtain the numerical results for surface magnetizations. At this point it is worth discussing whether or not the approximation may give reasonable results. Therefore, for the two special cases, the temperature dependences of surface and first-layer magnetizations are examined in Figs. 11 and 12, by introducing the four-layer approximation; we assume that from the third layer the magnetization of each layer

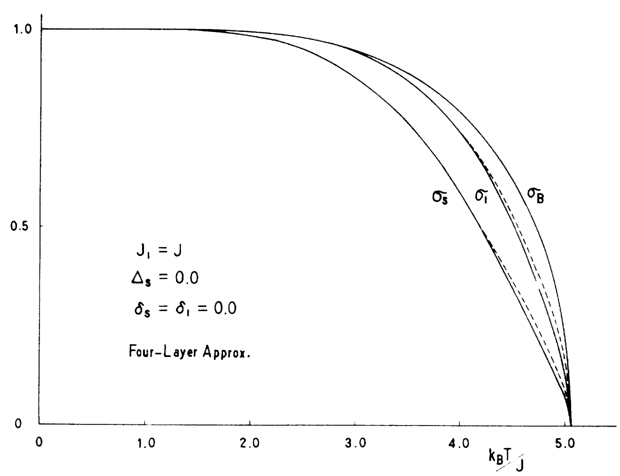

FIG. 11. Magnetization of surfaces, first layer, and bulk for the system with $\Delta_s=\Delta_1=0.0$ and $\delta_s=\delta_1=0.0$. Solid and dashed lines are obtained in the four- and three-layer approximations, respectively.

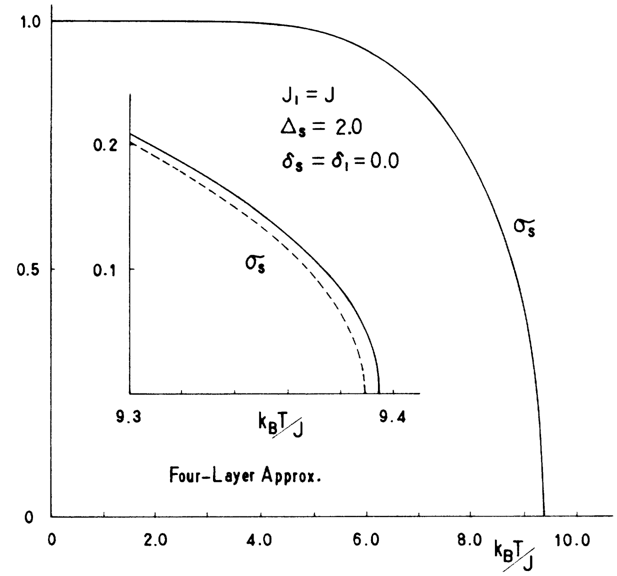

FIG. 12. Magnetization of surface for the system with $\Delta_s=2.0$, $\Delta_1=0.0$, and $\Delta_s=\delta_1=0.0$. The solid curve is obtained by the four-layer approximation. The dashed line in the insert corresponds to the three-layer approximation.

can be approximated by the bulk value, namely, $\sigma_3=\sigma_4=\cdots=\sigma_n=\sigma_B$. Figure 11 shows the thermal behavior of σ_s, σ_1, and σ_B for the system with $J_s=J$, $J_1=J$, and $\delta_s=\delta_1=0$ (Mills's model). In Fig. 11 solid and dashed lines correspond to the four- and three-layer approximations, respectively. The solid lines for σ_s and σ_1 deviate a little from the corresponding dashed lines near the bulk transition temperature. In particular, the linear temperature dependence of σ_s is more emphasized for the four-layer approximation than that for the three-layer approximation.

On the other hand, Fig. 12 is obtained for the system with $J_s=3J$, $J_1=J$, and $\delta_s=\delta_1=0$, corresponding to curve a in Fig. 9. Solid and dashed lines denote σ_s for four- and three-layer approximations, respectively. The magnetization curve of σ_s for the three-layer approximation is placed in the thickness of the solid line drawn. In the scale it is difficult to distinguish them, so that the behaviors near $T=T_c^s$ are given in the inset of the figure, taking a larger scale. As is seen from the inset the T_c^s value of the four-layer approximation is then given by $k_BT_c^s/J=9.395$, while for the three-layer approximation it is given by $k_BT_c^s/J=9.390$. Taking a better approximation, the transition temperature of surface ordering approaches the value ($k_BT_c^s/J=9.40$) obtained from the formulation of Sec. III.

Thus, the three-layer approximation gives a rather reasonable result for the thermal behavior of σ_s except in the temperature region very near $T=T_c^b$ (or T_c^s).

V. CONCLUSIONS

In this work we have studied the phase diagrams and the temperature dependence of surface magnetization for the semi-infinite simple-cubic spin-$\frac{1}{2}$ Ising ferromagnet with a surface amorphization by the use of the effective-field theory with correlations. Our results express a number of characteristic behaviors for the surface magnetism, such as the possibility of the surface reentrant phenomenon, large depressions of surface magnetization from those of pure ($\delta_s = \delta_1 = 0.0$) free crystalline surface, and so on, as shown in Sec. III and IV. Experimentally, however, it may not be so easy to observe the surface reentrant phenomenon in the system, since the J_s must be taken as a rather large value. Another way not to take such a large value of J_s for finding the surface reentrant phenomenon may be to apply the transverse field, as discussed in Ref. 11.

Finally, looking at the characteristic behavior of many surface magnetic properties, the study of a surface with an amorphous layer is extremely interesting and may open a new field of surface magnetism. We hope that our study will stimulate further experimental and theoretical work on the system considered here. A comparison of our work with experiment should be worthwhile.

APPENDIX

The coefficients L_i ($i = 1 - 8$), L, and R are defined by

$$\begin{aligned}
L_1 &= (\bar{s}_s)^3 \bar{c}_s \bar{c}_1 \tanh(\beta x)|_{x=0} ,\\
L_2 &= (\bar{c}_s)^2 (\bar{s}_s)^2 \bar{s}_1 \tanh(\beta x)|_{x=0} ,\\
L_3 &= (\bar{s}_s)^4 \bar{s}_1 \tanh(\beta x)|_{x=0} ,\\
L_4 &= (\bar{s})^3 (\bar{c})^2 \bar{c}_1 \tanh(\beta x)|_{x=0} ,\\
L_5 &= (\bar{s})^2 (\bar{c})^3 \bar{s}_1 \tanh(\beta x)|_{x=0} ,\\
L_6 &= (\bar{s})^4 \bar{c}\, \bar{s}_1 \tanh(\beta x)|_{x=0} ,\\
L_7 &= (\bar{s})^3 (\bar{c})^2 C_1 \tanh(\beta x)|_{x=0} ,\\
L_8 &= (\bar{s})^5 \bar{c}_1 \tanh(\beta x)|_{x=0} ,\\
L &= (\bar{s})^3 (\bar{c})^3 \tanh(\beta x)|_{x=0} ,
\end{aligned} \tag{A1}$$

and

$$R = (\bar{s})^5 \bar{c} \tanh(\beta x)|_{x=0} ,$$

where $\bar{s}_s$, $\bar{c}_s$, $\bar{c}_1$, $\bar{s}_1$, $\bar{s}$, and $\bar{c}$ are given by

$$\begin{aligned}
&\bar{s}_s = \langle \sinh(D\bar{J}_s) \rangle_r , \quad \bar{c}_s = \langle \cosh(D\bar{J}_s) \rangle_r ,\\
&\bar{c}_1 = \langle \cosh(D\bar{J}_1) \rangle_r , \quad \bar{s}_1 = \langle \sinh(D\bar{J}_1) \rangle_r ,\\
&\bar{s} = \sinh(DJ), \quad \bar{c} = \cosh(DJ) .
\end{aligned} \tag{A2}$$

These coefficients can be easily calculated by using a mathematical relation $e^{\alpha D} f(x) = f(x + a)$.

[1]See *Magnetic Properties of Low-Dimensional Systems,* edited by L. M. Falicov and J. L. Moran-Lopez (Springer, New York, 1986).

[2]D. T. Pierce, R. J. Celotta, J. Unguris, and H. C. Siegmann, J. Magn. Magn. Mater. **35**, 28 (1983).

[3]D. L. Mills, Phys. Rev. B **3**, 3887 (1971); **8**, 4424 (1973).

[4]E. F. Sarmento, R. A. Tahir-Kheli, I. P. Fittipaldi, and T. Kaneyoshi, in *Proceedings of Latin-America Colloquium of Surface Physics,* edited by Centro Latino-Americano de Fisica (Universidade Federal Fluminense, Brazil, 1980); J. M. Sanchez and J. L. Moran-Lopez, in *Magnetic Properties of Low-Dimensional Systems* (Ref. 1).

[5]K. Binder and P. C. Hohenberg, Phys. Rev. B **9**, 2194 (1974).

[6]K. Binder and D. P. Landau, Phys. Rev. Lett. **52**, 318 (1984).

[7]C. Tsallis, in *Magnetic Properties of Low-Dimensional Systems* (Ref. 1).

[8]See *Proceedings of the 4th International Conference on Rapidly Quenched Metals,* edited by T. Masumoto and K. Suzuki (Japan Institute of Metals, Japan, 1982).

[9]See *Magnetic Properties of Amorphous Metals,* edited by A. Hernando *et al.* (Elsevier, New York, 1987).

[10]T. Kaneyoshi, in *Physics of Magnetic Materials,* edited by M. Takahashi *et al.* (World Scientific, Singapore, 1987).

[11]T. Kaneyoshi and E. F. Sarmento, in *Magnetic Properties of Amorphous Metals* (Ref. 9).

[12]T. Kaneyoshi, I. Tamura, and E. F. Sarmento, Phys. Rev. B **28**, 6491 (1983).

[13]F. Zernike, Physica **7**, 565 (1940).

[14]T. Kaneyoshi, Phys. Rev. B **33**, 7688 (1986); J. Phys. Soc. Jpn. **55**, 1430 (1986); Phys. Rev. B **34**, 7866 (1986).

[15]T. Kaneyoshi, *Amorphous Magnetism* (Chemical Rubber Company, Boca Raton, 1984).

[16]K. Handrich, Phys. Status Solidi B **32**, K55 (1969).

[17]I. Tamura and T. Kaneyoshi, J. Phys. Soc. Jpn. **52**, 3208 (1983).

[18]T. W. Burkhard and E. Eisenviegler, Phys. Rev. B **16**, 3213 (1977).

[19]E. F. Sarmento and C. Tsallis, Phys. Rev. B **27**, 5784 (1983).

[20]T. Kaneyoshi, Phys. Rev. B **35**, 7180 (1987).

[21]T. Kaneyoshi, Phys. Status Solidi B **150**, 422 (1988).

[22]T. Kaneyoshi and I. Tamura, Solid State Commun. **51**, 67 (1984).