Magnetic properties and interface delocalization in the three-dimensional Ising model with defect-plane amorphization

A. Benyoussef, Y. El Amraoui, and A. El Kenz
Laboratoire de Magnétisme et Physique des Hautes Énergies, Faculté des Sciences, Boîte Postale 1014, Rue Ibn Battouta, Rabat, Morocco

T. Kaneyoshi
Department of Physics, Nagoya University, 464-01, Nagoya, Japan

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Magnetic properties and interface delocalization of the spin-$\frac{1}{2}$ Ising model on a cubic lattice with an amorphized defect plane that divides the system into two semi-infinite ones are investigated by the use of the effective-field theory. The global phase diagrams, which represent the connection between amorphized defect-plane order and wetting transitions (from partial to complete wetting), are given in the case of two equivalent semi-infinite systems (the same coupling) and in the case of different semi-infinite systems. The influence of the amorphization in these global phase diagrams is also studied. Moreover, magnetic properties which illustrate some interesting behavior for the amorphized systems are investigated.

I. INTRODUCTION

In the last decade, there has been an increasing number of experimental and theoretical works dealing with magnetic quantities of amorphous systems. Experimentally, structural information of amorphous metal-metal alloys including amorphous rare-earth–transition-metal and rare-earth–noble-metal alloys is very limited in comparison with those of metal-metalloid alloys. Most studies of amorphous magnetic alloys have been employed to alloys of transition metals (Fe,Co,Ni) with metalloid elements (B,C,Si,Ge,P), containing approximately 20 at. % of the latter.[1–6]

Theoretically, most works have been devoted to amorphous systems.[7–15] Among them, amorphization of the Ising ferromagnet with transverse field,[12] amorphous spinel ferrites,[13] the semi-infinite Ising model with surface amorphization,[14,15] and the amorphized interface problem.[16] In these works the authors used both effective-field theory[17] (EFT) and the lattice model of amorphous magnets in which the structural disorder is replaced by a random distribution of the exchange integral.[18]

In this paper we study a simple cubic spin-$\frac{1}{2}$ Ising ferromagnet with a defect plane amorphization by the use of EFT. We investigate the interface delocalization which corresponds to a wetting transition from partial to complete wetting. However, the critical behavior near surfaces, interfaces, and defects in various models has attracted considerable attention recently. Thus Svrakic'[19] and Mahajlovic' and Svrakic'[20] have used the real-space renormalization-group (RSRG) method to study interface delocalization in the two-dimensional (2D) Ising model. They have obtained that there is no interfacial depinning in the 2D Ising model, unless the bulk couplings at the two sides of the defect line are different. This result is consistent with the exact calculation.[21–23] Similar observations have been made for the three-dimensional (3D) Ising model by the RSRG method,[24,25] Landau phenomenological theory,[26,27] Monte Carlo simulation,[28] and other methods[25] such as the mean-field approximation (MFA) and finite-cluster approximation (FCA).

In Ref. 27, Iglói and Indekeu extend the work of Sevrin and Indekeu[26] to the case of unequal bulk couplings on the two sides of the defect plane. They give the qualitative shape of the phase diagrams in coupling-parameter space [bulk coupling (K), surface coupling ($K_{\parallel}$), and defect coupling ($K_{\perp}$)]. These phase diagrams will display very clearly the connection between defect-plane order and wetting phenomena. In their global phase diagrams, Iglói and Indekeu[27] have proposed a surface of first-order wetting transitions from partial to complete wetting for equal critical temperatures and surfaces of first order and critical wetting (second-order transition) separated by a line of tricritical wetting transitions for unequal critical temperatures.

Benyoussef and El Kenz[25] extend the work of Iglói and Indekeu[27] to other methods based on the two-state Ising model, namely, the MFA, FCA, and RSRG method. They give global phase diagrams which represent the connection between the defect-plane order and wetting phenomena. These phase diagrams are in agreement with those conjectured qualitatively by Iglói and Indekeu[27] in the case of two equivalent semi-infinite systems (the same coupling) and in the case of different semi-infinite systems.

The purpose of this paper is to extend the work of Benyoussef and El Kenz[25] to the case in which the defect plane is amorphized. We give, using EFT, global phase diagrams which represent the connection between amorphized defect-plane order and wetting phenomena. Also, we discuss the effect of amorphization in these global dia-

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grams. Finally, we investigate magnetic properties which illustrate some interesting behavior for the amorphized systems.

The outline of this paper is as follows. In Sec. II we present the formulation of this method in EFT and we investigate the global phase diagrams which represent the connection between amorphized defect plane order and wetting phenomena. In Sec. III we discuss the magnetic properties of the amorphized interface. Section IV contains our conclusions.

II. FORMULATION AND GLOBAL PHASE DIAGRAMS

We consider a simple cubic spin-$\frac{1}{2}$ Ising ferromagnet with a defect-plane amorphization as shown in Fig. 1. The Hamiltonian of the system is given by

$$H=-\sum_{\langle ij\rangle} J_{ij}\mu_i\mu_j \ , \tag{1}$$

where the summation is carried out only over nearest-neighbor pairs of spins, μ_i takes the values ± 1, and J_i is the exchange interaction. At one side of the defect plane, the bulk couplings have the values $K=-J/K_B T$ and at the other $K'=-J'/K_B T$ except for surface pairs which have distinct nearest-neighbor coupling constants $\bar{K}_\parallel=-\bar{J}_\parallel/K_B T$ and $K_\parallel=-J_\parallel/K_B T$ for the amorphized and crystalline surface, respectively. In order to describe the structural disorder in a simple way, the lattice model of amorphous magnets is used; the nearest-neighbor exchange interactions are given by independent random variables as

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

and define the parameter δ as

$$\delta=\frac{\Delta J_\parallel}{J_\parallel} \ , \tag{3}$$

which is often called the "structural fluctuation" in amorphous magnets.[17,28,29]

The two semi-infinite systems are coupled by a perpendicular interaction with coupling $K_\perp=-J_\perp/K_B T$ and have unequal critical temperatures T_c and T_c, respectively. Note that the critical bulk couplings are given by

$$K_b^c=\frac{J}{K_B T_c}=\frac{J'}{K_B T_c} \ .$$

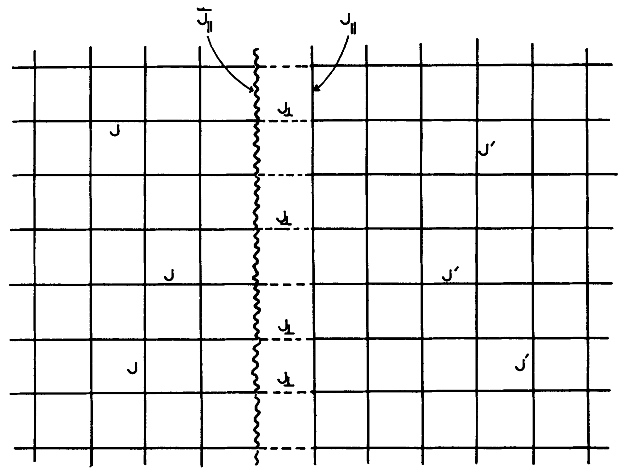

FIG. 1. Part of the two-dimensional cross section through the simple cubic Ising model with defect-plane amorphization. $J_\perp$ is the exchange interaction across the defect plane. $\bar{J}_\parallel$ and $J_\parallel$ are the amorphized surface interaction and crystalline surface interaction, respectively. All the interactions at the left of defect plane have the value J and those at the right side have the value J'.

The problem is now the evaluation of the mean value $\langle\mu_i\rangle$. The starting point for the statistics of our spin system is the exact Callen identity.[30] In this system we attribute the magnetizations σ and σ' to the volumes of sides 1 and 2, respectively. For surfaces 1 (amorphized) and 2 (crystallized) of the defect, the magnetizations as assumed to be $\sigma_\parallel$ and $\sigma_\parallel'$, respectively. Using the differential operator technique,[31] the magnetizations σ, σ', $\sigma_\parallel$, and $\sigma_\parallel'$ are given by

$$\sigma=\langle\langle \mu_{i(\in B)}\rangle\rangle_r=[\cosh(DJ')+\sigma\sinh(DJ)]^6\tanh(\beta x)|_{x=0} \ , \tag{4}$$

$$\sigma_\parallel=\langle\langle \mu_{i(\in\parallel 1)}\rangle\rangle_r=[\langle\cosh(D\bar{J}_\parallel)\rangle_r+\sigma_\parallel\langle\sinh(D\bar{J}_\parallel)\rangle_r]^4[\cosh(DJ)+\sigma\sinh(DJ)] \times[\cosh(DJ_\perp)+\sigma_\parallel'\sinh(DJ_\perp)]\tanh(\beta x)|_{x=0} \ , \tag{5}$$

$$\sigma_\parallel'=\langle\langle \mu_{i(\in\parallel 2)}\rangle\rangle_r=[\langle\cosh(DJ_\parallel)\rangle_r+\sigma_\parallel'\langle\sinh(DJ_\parallel)\rangle_r]^4[\cosh(DJ_\perp)+\sigma_\parallel\sinh(DJ_\perp)] \times[\cosh(DJ')+\sigma'\sinh(DJ')]\tanh(\beta x)|_{x=0} \ , \tag{6}$$

$$\sigma'=\langle\langle \mu_{i(\in B')}\rangle\rangle_r=[\cosh(DJ')+\sigma'\sinh(DJ')]^6\tanh(\beta x)|_{x=0} \ , \tag{7}$$

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. In the expression of $\sigma_\parallel$, these random bond averages are given by

$$\langle\cosh(D\bar{J}_\parallel)\rangle_r=\cosh(DJ_\parallel\delta)\cosh(DJ_\parallel) \ ,$$
$$\langle\sinh(D\bar{J}_\parallel)\rangle_r=\cosh(DJ_\parallel\delta)\sinh(DJ_\parallel) \ . \tag{8}$$

In order to obtain the thermal behavior of the magnetizations σ, σ', $\sigma_\parallel$, and $\sigma_\parallel'$, it is necessary to solve the above coupled equations. So we can have

$$\sigma=6M_1\sigma+20M_3\sigma^3+6M_5\sigma^5 \ , \tag{9}$$

$$\sigma_\parallel=A_1\sigma_\parallel+A_2\sigma+A_3\sigma_\parallel'+A_4\sigma^3+A_5\sigma_\parallel^2\sigma+A_6\sigma_\parallel^2\sigma_\parallel' + A_7\sigma'\sigma_\parallel\sigma_\parallel'+A_8\sigma_\parallel^4\sigma+A_9\sigma_\parallel^4\sigma_\parallel'+A_{10}\sigma_\parallel^3\sigma\sigma_\parallel' \ , \tag{10}$$

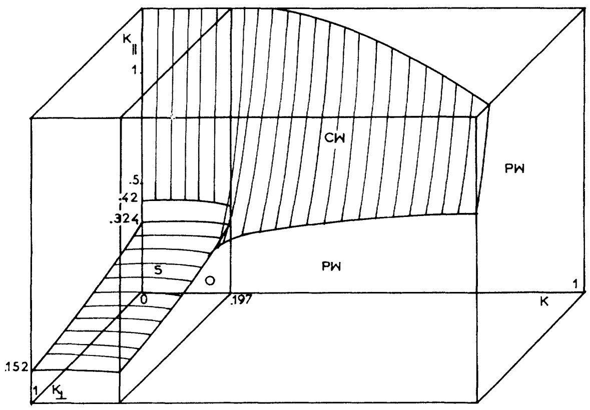

FIG. 2. Global phase diagram for wetting and amorphized surface transition, given by EFT, in the case $\alpha=1$. The wetting transition surface ($K>K_b^c=0.197$) is connected to the amorphized surface of defect-plane criticality ($K<K_b^c$). This surface for $K\geq K_b^c$ is given for a small value of $K_\perp$, i.e., for $0\leq K_\perp/K\leq 1$.

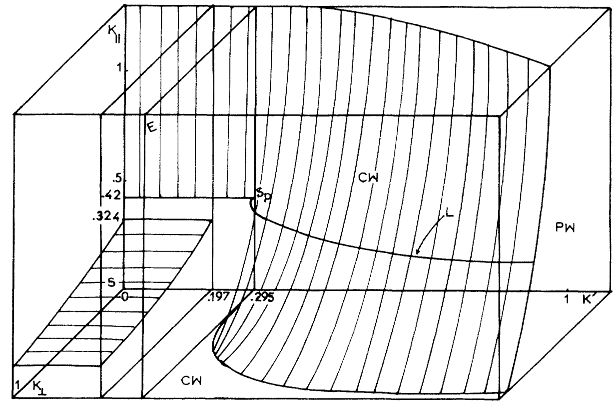

FIG. 3. Global phase diagram for wetting and amorphized surface transition, given by EFT, in the Ising model for $\alpha=1.5$. The critical surface of the defect plane stops at $K'=0.197$, except along $K_\perp=0$. On the wetting transition surface, the sheets of first-order wetting and critical wetting are separated by the critical line L.

$$\sigma'_\parallel=B_1\sigma'_\parallel+B_2\sigma'+B_3\sigma_\parallel+B_4\sigma'^3_\parallel+B_5\sigma'^2_\parallel\sigma'+B_6\sigma'^2_\parallel\sigma_\parallel+B_7\sigma'\sigma_\parallel\sigma'_\parallel+B_8\sigma'^4_\parallel\sigma'+B_9\sigma'^4_\parallel\sigma_\parallel+B_{10}\sigma'^3_\parallel\sigma'\sigma_\parallel\ , \quad (11)$$

$$\sigma'=6N_1\sigma'+20N_3\sigma'^3+6N_5\sigma'^5\ . \quad (12)$$

where the coefficients M_i, A_i, B_i, and N_i are given in the Appendix. Using Eqs. (8)–(12), we can study the two cases of equal ($K=K'$) and unequal ($K\neq K'$) bulk couplings. Thus we give the corresponding global phase diagrams which represent the connection between surface phase transitions and the phase transition from partial to complete wetting. In both cases we take $\delta=0.8$.

Figure 2 shows the global phase diagram of equal critical temperature ($K_1=K_2=K$). The order-disorder phase diagram, in ($K,K_\parallel,K_\perp$) space, is obtained for $K<K_b^c=0.197$. Note that $K_b^c=0.197$ is the critical bulk coupling given by EFT and is better than that obtained by MFT ($K_b^c=0.167$) compared to the exact result (0.222).[32] In the plane $K_\perp=0$, we find the line of surface amorphization criticality of the semi-infinite simple cubic spin-$\frac{1}{2}$ Ising ferromagnet with a surface amorphization, which terminates at the special transition point S_p. Below this line, at $K_\perp=0$, the line of the free crystalline surface appears. For $K_\perp\neq 0$ we can distinguish the sur-

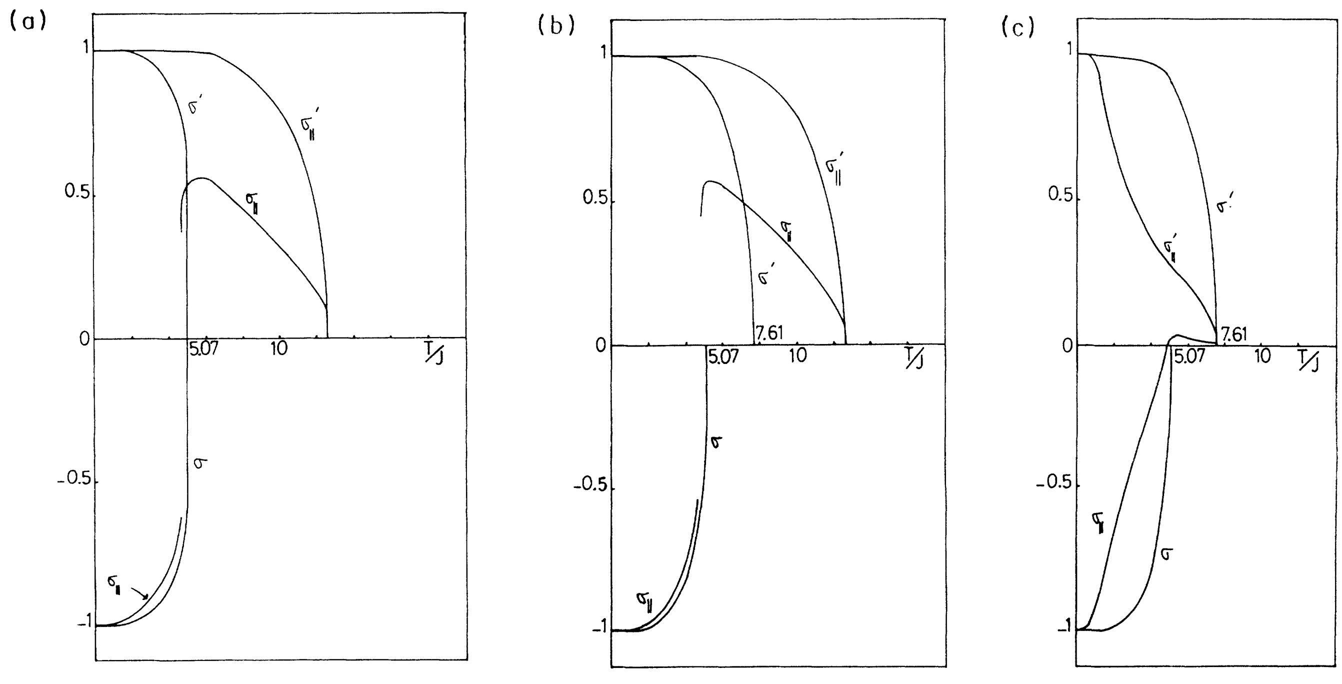

FIG. 4. Temperature dependences of $\sigma_\parallel$, $\sigma'_\parallel$, σ, and σ' for the system in both cases (a) $\alpha=1$ and (b), (c) $\alpha=1.5$. The wetting transition surface is first-order wetting [(a) and (b)] while in (c) it is second-order wetting.

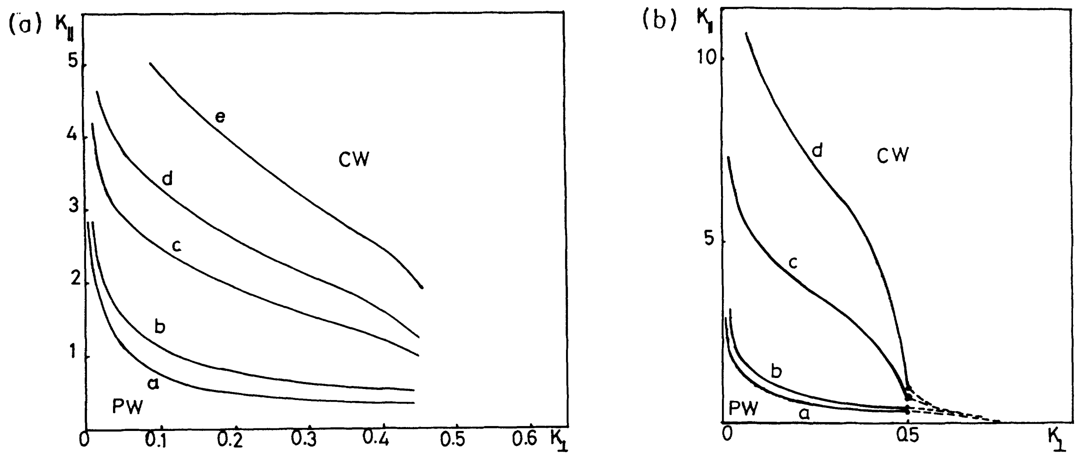

FIG. 5. Phase diagrams in the $(K_\parallel, K_\perp)$ plane, for a fixed value of $K=0.5$ and selected values of δ, in both cases (a) $\alpha=1$ and (b) $\alpha=1.5$. In (a), curves a, b, c, d, and e are obtained for $\delta=0$, 0.5, 0.8, 0.85, and 0.9, respectively. In (b), curves a, b, c, and d are for $\delta=0$, 0.5, 0.9, and 0.95, respectively. Solid and dashed lines indicate first- and second-order wetting transition lines, respectively. The solid dots denote the tricritical points.

faces of surface (S), ordinary (O), extraordinary transition (E), and the multicritical line of special transitions.[25,27,33,34] Contrary to the case $K_\perp=0$, amorphization and crystalline surfaces order, for $K_\perp \neq 0$, at the same temperature. So the surface (S) is the same for surfaces (1) and (2). For $K > K_b^c = 0.197$, the phase diagram is completed by a surface of wetting transitions. This surface transition separates the partial wetting region ($\sigma < 0$, $\sigma_\parallel < 0$, $\sigma'_\parallel > 0$, $\sigma' > 0$) and the complete wetting region ($\sigma < 0$, $\sigma_\parallel > 0$, $\sigma'_\parallel > 0$, $\sigma' > 0$). This transition is a first-order wetting phase transition. Indeed, the amorphized surface magnetization $\sigma_\parallel$ becomes discontinuous through the surface wetting transition.

In the second case ($K \neq K'$), we restrict ourselves to the value of $\alpha=1.5$ ($\alpha=K/K'$). For $K' < K'_c = K_b^c = 0.295$ and in the plane $K_\perp=0$, we find the usual line of amorphized surface criticality which terminates at the special transition point as shown in Fig. 3. For $K_\perp \neq 0$ the surface of defect-plane criticality ($K < K_c = 0.197$) terminates at $K = K_c$. The wetting phase transition occurs at $K' > K'_c$. However, we find the first-order wetting surface and the critical wetting surface. These surfaces are separated by a tricritical line. Note that through the critical wetting surface, the amorphized surface magnetization $\sigma_\parallel$ is continuous.

In order to display the behavior of the magnetization of the amorphized surface in the defect plane, in both cases $K = K'$ and $K = 1.5K'$, we give the curves of $\sigma_\parallel$ in Fig. 4. In the first case, we take $K_\perp = 0.1$ and $K_\parallel = 4K$. At the wetting transition temperature, the magnetization $\sigma_\parallel$ becomes discontinuous and vanishes at the same surface transition temperature as the crystallized surface $\sigma'_\parallel$ for $T > T_b^c = 5.073J$. This behavior is also given in the second case $K = 1.5K'$ [Fig. 4(b)]. Furthermore, in Fig. 4(c) ($K = 1.5K'$), in which we take $K_\perp = 0.1$ and $K_\parallel = 0.1$ K, the magnetization $\sigma_\parallel$ is continuous at the critical wetting transition temperature. As in Figs. 4(a) and 4(b), the magnetizations $\sigma_\parallel$ and $\sigma'_\parallel$ vanish at the same surface critical temperature in the order-disorder phase diagram.

In Fig. 5 we show the influence of amorphization in both cases $K = K'$ and $K \neq K'$. For this, we take a fixed value of K ($K=0.5$) for selected values of δ. Thus, in the $(K_\parallel, K_\perp)$ plane (Fig. 5), for a fixed value of $K_\perp$, the wetting transition temperature (from partial to complete wetting) increases with δ. Then, in $(K, K_\parallel, K_\perp)$ space, the surfaces of the wetting transitions are superimposed. The influence of amorphization is very important in the first-order wetting transitions in both cases $K = K'$ [Fig. 5(a)] and $K \neq K'$ [Fig. 5(b)]. Moreover, for $K_\parallel = 0$, all the critical wetting lines join at the same point in the $K_\perp$ axis [Fig. 5(b)]. Consequently, for $K_\parallel = 0$, there exists only one critical wetting line in $(K_\parallel, K_\perp)$ space.

III. MAGNETIC PROPERTIES

In this section we examine the phase diagram, which illustrates some interesting behavior of the amorphized surface. Thus, using Eqs. (9)–(12), the amorphized surface ordering temperature T/K_BJ is plotted as a function of δ.

In Fig. 6(a) the changes of T_c/K_BJ versus the values of δ are depicted for the three values of $J_\perp$ [$J_\perp = 1.1$, $0.1J$, and 0]. The values of $J_\parallel$ and α are fixed as $J_\parallel = 8J$ and $\alpha = 1$, respectively. In the semi-infinite case ($J_\perp = 0$), the surface reentrant phenomenon cannot be obtained. This result is in accordance with that given by Kaneyoshi.[15] In this work[15] the reentrant phenomenon appearing for J_s ($J_\parallel$) becomes larger than bulk J and the perpendicular interaction between amorphized surface and bulk is taken as a value smaller than bulk J. In our work this perpendicular interaction is equal to J. Also, the reentrant phenomenon is not observed in the other case $J_\perp = 1.1J$ and $0.1J$. Indeed, in the three-dimensional Ising model with an amorphized interface, this phenomenon appears when the interface exchange parameter becomes larger than that of the bulk and the perpendicular exchange interaction, between the amorphized interface and the bulk in two sides, is taken as a value smaller than the bulk exchange interaction.[16]

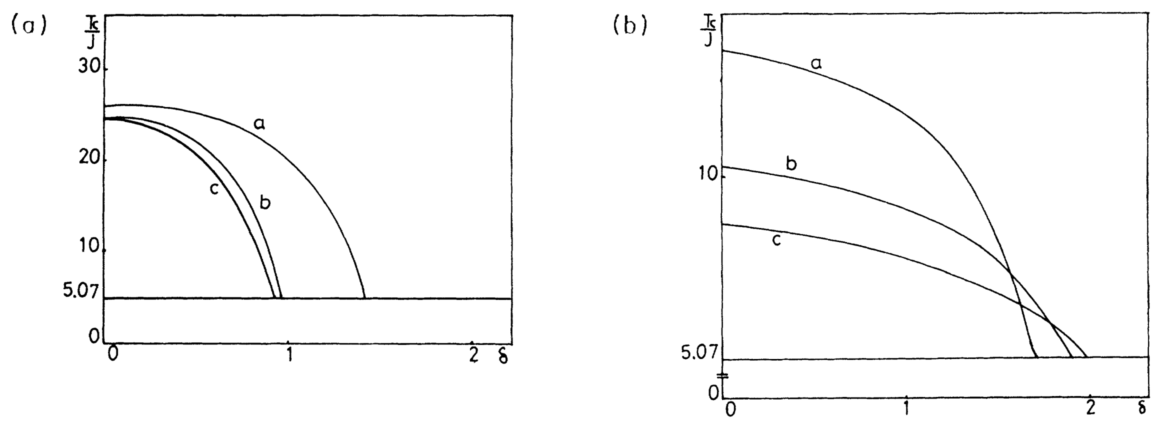

FIG. 6. Phase diagrams in the $(T_c/K_BJ,\delta)$ plane in the case $\alpha=1$. In (a), $J_\parallel=8J$ and curves a, b, and c are given by $J_\perp=1.1J$, $0.1J$, and 0, respectively. In (b), $J_\perp$ is fixed as $J_\perp=J$ and curves a, b, and c are given by $J_\parallel=4J$, $3J$, and $2.5J$.

In Fig. 6(b), T_c/K_BJ is depicted for three selected values of $J_\parallel$ when $J_\perp$ is fixed as $J_\perp=J$. We remark that, at $\delta=0$, the transition temperature of the interface increases with $J_\parallel$. On the other hand, at the bulk critical temperature the critical values of δ decrease when $J_\parallel$ increases. Also, the reentrant phenomenon is not observed.

IV. CONCLUSION

In this work we have studied a three-dimensional Ising model with defect-plane amorphization by the use of effective-field theory. In the first part, we investigated the global phase diagrams, which represent the connection between amorphized defect-plane order and wetting phenomena, in the cases $K=K'$ and $K\neq K'$. These phase diagrams are in accordance with those given qualitatively by Iglói and Indekeu[27] and by three approximate methods by Benyoussef and El Kenz.[25] Indeed, we formed the first-order wetting transition in the case $K=K'$ and first-order wetting and critical wetting surfaces and a critical wetting line in the case $K\neq K'$. Furthermore, we have also studied how amorphization affects these global phase diagrams.

Finally, we have investigated some interesting behaviors of the amorphized interface. Thus the reentrant phenomenon in the $(T/K_BJ,\delta)$ plane is studied. Our results are in agreement with others given, by Kaneyoshi,[15] in the semi-infinite system.

APPENDIX

$$A_1=4\langle\cosh(D\bar{J}_\parallel)\rangle_r^3\langle\sinh(D\bar{J}_\parallel)\rangle_r\cosh(DJ)\cosh(DJ_\perp)\tanh(\beta x)|_{x=0}\ ,$$

$$A_2=\langle\cosh(D\bar{J}_\parallel)\rangle_r^4\sinh(DJ)\cosh(DJ_\perp)\tanh(\beta x)|_{x=0}\ ,$$

$$A_3=\langle\cosh(D\bar{J}_\parallel)\rangle_r^4\cosh(DJ)\sinh(DJ_\perp)\tanh(\beta x)|_{x=0}\ ,$$

$$A_4=4\langle\cosh(D\bar{J}_\parallel)\rangle_r\langle\sinh(D\bar{J}_\parallel)\rangle_r^3\cosh(DJ)\cosh(DJ_\perp)\tanh(\beta x)|_{x=0}\ ,$$

$$A_5=6\langle\cosh(D\bar{J}_\parallel)\rangle_r^2\langle\sinh(D\bar{J}_\parallel)\rangle_r^2\sinh(DJ)\cosh(DJ_\perp)\tanh(\beta x)|_{x=0}\ ,$$

$$A_6=6\langle\cosh(D\bar{J}_\parallel)\rangle_r^2\langle\sinh(D\bar{J}_\parallel)\rangle_r^2\cosh(DJ)\sinh(DJ_\perp)\tanh(\beta x)|_{x=0}\ ,$$

$$A_7=4\langle\cosh(D\bar{J}_\parallel)\rangle_r^3\langle\sinh(D\bar{J}_\parallel)\rangle_r\sinh(DJ)\sinh(DJ_\perp)\tanh(\beta x)|_{x=0}\ ,$$

$$A_8=\langle\sinh(D\bar{J}_\parallel)\rangle_r^4\sinh(DJ)\cosh(DJ_\perp)\tanh(\beta x)|_{x=0}\ ,$$

$$A_9=\langle\sinh(D\bar{J}_\parallel)\rangle_r^4\cosh(DJ)\sinh(DJ_\perp)\tanh(\beta x)|_{x=0}\ ,$$

$$A_{10}=4\langle\cosh(D\bar{J}_\parallel)\rangle_r\langle\sinh(D\bar{J}_\parallel)\rangle_r^3\sinh(DJ)\sinh(DJ_\perp)\tanh(\beta x)|_{x=0}\ ,$$

$$M_1=\sinh(DJ)\cosh^5(DJ)\tanh(\beta x)|_{x=0}\ ,$$

$$M_3=\sinh^3(DJ)\cosh^3(DJ)\tanh(\beta x)|_{x=0}\ ,$$

$$M_5=\sinh^5(DJ)\cosh(DJ)\tanh(\beta x)|_{x=0}\ .$$

The coefficients $B_i(N_i)$ can be deduced from $A_i(M_i)$ by replacing $\bar{J}_\parallel$ and J by $J_\parallel$ and J', respectively.

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