Title

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Journal

Physical Review B, 51(189)

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Publication Date

1994-09-01

LBL-36153
UC-404
Preprint

Lawrence Berkeley Laboratory

UNIVERSITY OF CALIFORNIA

Materials Sciences Division

Submitted to Physical Review B

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September 1994

Prepared for the U.S. Department of Energy under Contract Number DE-AC03-76SF00098

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This work is supported in part by the Department of Energy, Basic Energy Sciences, Materials Sciences Division, under Contract No. DE-AC03-76SF00098, and the Office of Naval Research under Contracts No. N00014-90-5-1457 and N00014-94-1-0162.

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A MONTE CARLO STUDY OF MAGNETIC ORDER AT FERROMAGNETIC AND ANTIFERROMAGNETIC SURFACES: IMPLICATIONS FOR SPIN-POLARIZED PHOTOELECTRON DIFFRACTION

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ABSTRACT

We have used Monte Carlo simulations on simple cubic Ising lattices with modified surface interaction parameters to model phenomenologically the temperature dependence of magnetic order near ferromagnetic and antiferromagnetic surfaces. These results are also discussed in connection with previous experiments suggesting surface-specific magnetic transition temperatures for semi-infinite systems, with special emphasis on spin-polarized photoelectron diffraction as a probe of short-range magnetic order. The calculated spin-spin correlation functions show no evidence of a high-temperature transition in short-range magnetic order. However, over a plausible range of choices for the surface interaction parameters, these correlation functions do show distinct surface transitions in long-range magnetic order that can be well above $T_{N,bulk}$ for antiferromagnets (both frustrated and non-frustrated) and well above $T_{C,bulk}$ for ferromagnets. Thus, prior spin-polarized photoelectron data

from antiferromagnetic $KMnF_3$ and MnO may be explainable via such surface magnetic transitions, although further theoretical and experimental work is necessary to make this connection quantitative and definitive.

PACS numbers: 75.30.Pd, 64.60.Cn, 05.70.Fh

I INTRODUCTION

The nature of magnetic order near surfaces and interfaces is a topic of high current interest, with experimental observations or theoretical predictions of Curie temperatures which may depend either on the thickness of an epitaxial ferromagnetic layer or may vary from the surface layer inward for a semi-infinite sample of homogeneous composition [1]. The temperature dependence of surface magnetic order is thus a key component of surface magnetism, particularly for systems of nanometer scale for which the fraction of surface atoms can become appreciable. Previous theoretical modelling of this temperature dependence has been carried out primarily for the surfaces of ferromagnetic systems using Monte Carlo methods and cluster variation methods [2,3]. In this paper, we have applied Monte Carlo modelling to both ferromagnetic and antiferromagnetic surfaces, for the later case considered systems without and with frustrated next-nearest-neighbor interactions, explored a broader range of relative interaction parameters, and considered the relationship of these results to both prior theoretical calculations [2,3] and previous experimental data suggesting surface magnetic order behavior different from the bulk [4-9,11-12]. Special emphasis is placed on prior experimental studies by spin-polarized photoelectron diffraction [4-9]. We first review the experimental data which appear to show a surface magnetic transition temperature different from the bulk for semi-infinite samples and the previous theoretical modelling of these phenomena, and then turn to our theoretical simulations of such effects.

I.1 Spin-polarized photoelectron diffraction studies on antiferromagnetic systems

Spin-polarized photoelectron diffraction (SPPD) has been proposed as a probe for studying short-range magnetic order in both ferromagnetic and antiferromagnetic materials [4-10]. In its simplest form, SPPD makes use of multiplet-split core-level binding energies as internally-referenced sources of spin-polarized electrons, with no external spin detector then being necessary. But if an external spin detector is used with a speciman possessing a net magnetization [9] and/or spin-orbit-split levels are excited by circularly-polarized radiation [10], SPPD can be related to an external axis of electron spin polarization. Like the much more developed technique of photoelectron diffraction (PD) without spin resolution [10], SPPD will be primarily sensitive to the first few spheres of neighbors surrounding an emitter [9,10]. The fact that SPPD must be carried out at electron kinetic energies of only 50-150 eV in order to have sufficiently strong magnetic scattering also implies high surface sensitivity [9,10], so magnetic properties in the first few layers below a surface are preferentially investigated using this technique. Thus, the change in orientation of magnetic moments in ferromagnetic or antiferromagnetic materials can in principle be studied by analyzing the spin-polarized photoelectron diffraction intensities above a surface as a function of temperature. An experimental quantity which has been used to detect changes in magnetic order is the so-called spin asymmetry S [5-9]:

$$S = 100[(R_{LT} - R_{HT})/R_{HT}]\% \qquad (1)$$

where R_{HT} represents the (spin-up):(spin-down) intensity ratio for the highest temperature data point in the series (assumed to be in the fully disordered or paramagnetic limit), and R_{LT} represents the same ratio for any lower temperature data point below R_{HT}. The spin asymmetry is thus defined to go to zero at the limit of HT.

The first experimental study by SPPD was reported by Sinkovic and co-workers [4]. They studied the antiferromagnetic surface of $KMnF_3$(110) through the temperature dependence of the spin-up and spin-down multiplet peaks associated with Mn 3s core emission and found that the experimental spin asymmetry $S_{expt.}$ went through an abrupt transition at a temperature that was about 2.7 times higher than the bulk Néel temperature. They interpreted their results as an abrupt reduction in short-range magnetic order (SRMO) at this transition temperature, even though long-range order has completely disappeared well below this temperature. Subsequently Hermsmeier et al. [6,8] used SPPD to study another antiferromagnetic surface, MnO(001), and saw a similar effect in the spin asymmetries, but in this case with the transition temperature about 4.5 times higher than the bulk Néel temperature. Fig. 1 summarizes some of this experimental data for MnO. The spin asymmetry for this photoelectron emission direction (along the surface normal) exhibits a small, but reproducible peak with a value of 33% at 120 K (which is also the bulk Neel temperature ($T_{N,bulk}$)). $S_{expt.}$ then decreases monotonically up to about 540 K to a value of about 21%, probably due to Debye-Waller effects. Over the narrow range 540-580 K, it drops rapidly from 21% to about 7%, again a fully reproducible effect [8]. For temperatures above 580 K, $S_{expt.}$ again decreases more slowly, probably due to simple Debye-Waller effects [8]. This SPPD study of MnO again concluded that a sharp SRMO transition occurred at a temperature much higher than the bulk Néel temperature. However, it was not possible in either of these prior SPPD studies to fully rule out a surface magnetic transition in long-range order that, through the concomitant abrupt change in short-range order, would also affect the spin asymmetry seen in SPPD. Some sensitivity of SPPD to bulk long-range order is also suggested by the peak near T_N in Fig. 1.

Prior theoretical analyses of SPPD have not dealt specifically with the statistical mechanics of spins near surfaces beyond considering what configuration averages would be sensed by the experiment. Sinkovic and Fadley [5] considered only zero-temperature SPPD to simulate the spin-polarized photoelectron diffraction intensities from a small cluster. Friedman and co-workers [7] subsequently extended this theory to finite temperature, showing explicitly how the spin-polarized photoelectron diffraction intensity depends on averages of spin-spin correlation functions. They showed that the average of intensities at finite temperature is well approximated by the intensity calculated for a single configuration with all spins parallel (or anti-parallel) to the emitter, but with effective scattering phase shifts involving averages over spin-spin correlation functions. They also showed that spin-spin correlation functions of the usual form and with the bulk transition temperature could not explain the step-like feature at the high temperature, even though the spin-spin correlation functions themselves showed abrupt changes near the bulk transition temperature. Finally, it has been shown that the overall change in $S_{expt.}$ in going over the high-temperature transition (e.g., 14% in MnO) is semi-quantitatively predicted by spin-dependent diffraction calculations based only on results for zero-temperature and a high-temperature paramagnetic limit [8,9].

I.2 Other experiments on ferromagnetic systems

Two ferromagnetic surfaces for which the Curie temperature seems to be higher than that of the bulk have also been studied using other experimental techniques [11,12]. Rau and Eichner [11a] first found evidence for ferromagnetic order at Gd surfaces above the bulk Curie temperature using deuteron electron capture spectroscopy. Weller et al. [11b] have used spin-polarized low-energy-electron diffraction to study epitaxial Gd(0001) films on W(110) and subsequently concluded that the surface transition temperature lies 22K above the bulk Curie temperature of 293 K. This result has been confirmed by Tang et al. [11c] using spin resolved electron spectroscopy, with a surface Curie temperature 60 ± 2 K above the bulk. In addition, Rau et al. [12] have also previously studied the surface of Tb(0001) using electron capture, and have found a surface transition temperature that is 30 K above the bulk Curie temperature of 220 K.

I.3 Prior theoretical modelling of surface magnetic phase transition

Prior statistical mechanical simulations that predict surface transitions at significantly higher temperatures than the bulk have mainly been performed on simple cubic ferromagnetic lattices with nearest-neighbor interactions only [2,3]. Binder and Hohenberg first studied the surface behavior of a semi-infinite simple-cubic Ising ferromagnet with nearest-neighbor interactions which could be modified in the surface layers with respect to that in the bulk; they did this both in mean-field theory and by means of high-temperature-series expansions [2(a)], and found that, for sufficiently enhanced surface coupling, the surface ordered at a higher temperature than the bulk, and behaved like a two-dimensional (2D) Ising model above the bulk order temperature. The ranges over which the 2D behavior was seen were for the surface exchange integral $J_s > 1.25$ times the bulk exchange integral J_b in mean-field theory, and $J_s > 1.6\ J_b$ from high-temperature-series expansions. Binder and Landau later studied a simple cubic Ising ferromagnet with nearest-neighbor ferromagnetic exchange interaction J_b in the bulk and a nearest-neighbor antiferromagnetic exchange interaction J_s between surface spins using Monte Carlo simulations [2(b)]. They investigated the ordering for a variety of values of $J_s/J_b < 0$ and for various temperatures and found that for $J_s < -2.01\ J_b$ the surface transition occured at a higher temperature than the bulk transition. By studying the magnetization profile of the system, they also found that the magnetization under the surface layer was hardly affected by the antiferromagnetic ordering in the surface and that the surface layer would be a very good approximation to a two-dimensional Ising antiferromagnet. More recently, Landau and Binder [2(d)] reported more precise results of extensive Monte Carlo simulations of phase transitions and critical behavior at the surface of a simple cubic Ising ferromagnetic model with nearest-neighbor exchange interactions only. By studying profiles of the magnetization and internal energy as a function of the distance from the surface, they extracted surface and bulk properties as a function of temperature and surface exchange interaction J_s. They found that the surface transition temperature $T_{C,surf}$ exceeded the bulk critical temperature $T_{C,bulk}$ when J_s/J_b was greater than 1.52. Using the cluster variation method, Sanchez and Moran-Lopez [3] have also shown that a surface transition takes place at a higher temperature than the bulk when J_s/J_b is greater than 1.47 for (100) surfaces of simple cubic lattices in the cubic approximation and greater than 2.25 and 1.778 for (100) surfaces and (111) surfaces of face-centered-cubic structures in the tetrahedron approximation respectively.

As reviewed above, prior theoretical work primarily deals with the surface behavior of simple cubic ferromagnetic Ising lattices with nearest-neighbor exchange interactions only, without considering the case of simple cubic frustrated antiferromagnetic Ising lattices. Thus, in this paper, we will study the surface and near surface behavior of both ferromagnets and antiferromagnets (both frustrated and unfrustrated) in order to understand further of the spin statistics behind such high-temperature transitions. Since SPPD, as well as electron capture by deuterons [11a, 12] and other surface-sensitive electron spectroscopies [11b, c] are sensitive to spin-spin correlation functions on and near the surface, we will here also explore intra-layer, inter-layer and overall spin-spin correlation functions on and near the surface in a simple Ising model with both nearest-neighbor (nn) and next-nearest-neigbor (nnn) interactions. We will also investigate the effects of varying degrees of enhancement of surface interactions on both surface and near-surface behavior, and the effects of varying relative strengths of next-nearest-neighbor interactions on the general behavior of near surface spin-spin correlation functions.

In section II, we will give a brief discription of the theoretical model and simulation method used. In section III, our detailed results and analyses are presented. Here, we first study the ferromagnetic and antiferromagnetic Ising lattices with only nn interaction, and then investigate frustrated antiferromagnetic Ising lattices with both nn and nnn interactions. Finally, In section IV, we draw our conclusions and also make a few further remarks on the degree of applicability of such modelling and promising directions for future work.

II METHODS

II.1 Ising Model with nn and nnn Interactions

It is expected that magnetic order and critical behavior on a surface or near a surface will be different from that of the bulk for purely geometric reasons, namely the absence of the neighboring atoms above the surface, and the resultant lowering of the surface coordination number. However, changes may also occur due to modified exchange interactions, and these changes may in turn be enhanced by surface relaxations or reconstructions of atomic positions (although we will not explicitly consider such geometry changes here). For example, Scholl et al. [13] have shown that the surface exchange integral J_s can be changed dramatically with respect to the bulk exchange integral J_b in different surface environments. They found that, by depositing a submonolayer of Fe on a clean Ni-Fe surface, J_s can be increased to as much as 3 times J_b [13]. A final surface effect is the reduction of the bandwidth and associated enhancement of local moments. This could be an important effect in itinerant models of surface magnetism.

We here adopt a three-dimensional simple-cubic Ising model in order to be able to account phenomenologically for changes in surface interaction parameters, as illustrated in Fig. 2. The Hamiltonian used is:

$$H = - J_s(nn)\Sigma_{nn,surf}S_iS_j - J_b(nn)\Sigma_{nn,bulk}S_iS_j - J_s(nnn)\Sigma_{nnn,surf}S_iS_j - J_b(nnn)\Sigma_{nnn,bulk}S_iS_j \qquad (2)$$

where $S_{i,j} = \pm 1$, $J_s(nn)$ and $J_s(nnn)$ are the nearest-neighbor(nn) and next-nearest-neighbor(nnn) exchange integrals respectively in the surface layer, and $J_b(nn)$ and $J_b(nnn)$ are the corresponding quantities in the "bulk" layers below the surface. The <u>interlayer</u> coupling between surface and bulk is assumed to be controlled by $J_b(nn)$ and $J_b(nnn)$, although the interlayer interactions could in general vary near the surface as well. The nnn exchange interactions are included only when studying the frustrated antiferromagnetic systems.

II.2 Monte Carlo Simulation

A standard single-flip Monte Carlo method [14, 15] was used. Since SPPD and other probes of surface magnetic order are primarily sensitive to short-range spin-spin correlations [9,10,11,12], the long-range effects in correlation length are not of primary interest here. Also, surface perturbations on underlying layers were found to be negligibly small after about the third layer for the choices of parameter used here. Thus, most of the simulations were performed on a 10-layer lattice of spins with 40x40 spins in each layer instead of thicker, and much more time consuming, lattices. However, a few calculations were done on a 40x40x40 lattice to be sure that the results reported here were not significantly influenced by finite-size effects. Periodic boundary conditions were imposed in the directions parallel to the surfaces, and free boundary conditions were used in the directions normal to the top surface and the bottom surface, which are equivalent to each other. Spin-spin correlation functions were calculated intra-layer, inter-layer and over all spins in the lattice for the first five layers near the surface. The number of iterations used per site was 3×10^3, and found to be adequately equilibrated in tests on both ferromagnetic and antiferromagnetic systems with 1.5×10^5 iterations per site. Our correlation function results were checked against high-temperature series expansions and exact results for a two-dimensional limit, and excellent agreement was found. Also, we checked the critical behaviors of a two-dimensional 40x40 square lattice and the 40x40x10 simple cubic lattice with nearest-neighbor exchange interactions under periodic boundary conditions in all directions and found that the critical temperatures T_C are very close to 2.269 $J_b(nn)/k_B$ [16, 17] and 4.51 $J_b(nn)/k_B$ [17, 18], which correspond to the well known T_C values for two-dimensional and three-dimensional homogeneous cases respectively.

III RESULTS

III.1 Ferromagnetic and Antiferromagnetic Ising Lattices with nn Interactions

In this section we present results for spin-spin correlation functions in the first five layers near a ferromagnetic surface with different relative surface:bulk interactions. The calculations were carried out on a simple cubic Ising ferromagnetic system with nearest-neighbor interactions only.

In Fig. 3, we show the intra-layer (Fig. 3(a)) and inter-layer (Fig. 3(b)) spin-spin correlation functions between nearest neighbors calculated for the first five layers near the surface with $J_s(nn) = J_b(nn) = 1.0$ (in units of k_BT). Since $J_s(nn)$ is equal to $J_b(nn)$, the only surface effect is reduced coordination number. Both of these figures show that the intra-layer and inter-layer spin-spin correlation functions fall off abruptly near the same bulk Curie temperature $T_{C,bulk}(\approx 4.5\ J_b(nn)/k_B)$ and decrease smoothly at higher temperatures. Although these correlation functions behave very much the same for all layers, the transition does occur at a slightly lower temperature in the surface layer, and then in the second layer, with the third-to-fifth layers being essentially identical and fully bulklike in their behavior. These small differences are expected from the lower surface coordination number and the resulting weaker surface order.

In Fig. 4, we now compare the spin-spin correlation functions for different relative strengths of surface exchange $J_s(nn)/J_b(nn) = 1.00$, 1.90, 2.75, 4.35, and 6.0, with the corresponding spin-spin correlation functions calculated for a bulk system based upon a 40x40x10 lattice with $J_b(nn) = 1.0$ (denoted as "Bulk" in the figure). The intra-layer spin-spin correlation functions in the surface layer are shown in Fig. 4(a) and the inter-layer spin-spin correlation functions between the surface and the 2nd layer are shown in Fig. 4(b). Intra-layer spin-spin correlation functions in the 2nd layer appear in Fig. 4(c). The vertical dashed line indicates the bulk Curie temperature ($T_{C,bulk}$). The surface critical temperature ($T_{C,surf}$) corresponding to the abrupt step-like falloff of the intra-layer spin-spin correlation functions in Fig. 4(a) is found to increase rapidly with an increase in the surface exchange interaction. When $J_s(nn)/J_b(nn) = 2.75$, $T_{C,surf}(\approx 6.3\ J_b(nn)/k_B)$ is about 1.4 times $T_{C,bulk}(\approx 4.5\ J_b(nn)/k_B)$, but when $J_s(nn)$ is increased to 6.0, $T_{C,surf}(\approx 13.4\ J_b(nn)/k_B)$ increases to about 3 times $T_{C,bulk}$. However, Fig. 4(b) shows that the spin-spin correlations between the surface and the second layer are affected very little by these changes in surface exchange interactions. Finally, the intra-layer spin-spin correlation curves for the second layer in Fig. 4(c) are much closer to each other for these five different values of $J_s(nn)/J_b(nn)$ and do not differ very much from the curve for the bulk case: thus, changing $J_s(nn)$ does not significantly affect the spin arrangements in the second layer.

The two-dimensional critical temperature $T_{C,2d}$ for a simple square ferromagnetic lattice is equal to $2.269 \cdot J_s(nn)/k_B$, where $J_s(nn)$ here corresponds to the exchange integral in the two-dimensional case [16,17]. This relationship thus leads directly to $T_{C,2d} = 6.24\ J_b(nn)/k_B$ for $J_s(nn)/J_b(nn) = 2.75$ and $13.61\ J_b(nn)/k_B$ for $J_s(nn)/J_b(nn) = 6.0$. Our calculated values of $T_{C,surf}$ for both of these cases (about $6.3\ J_b(nn)/k_B$ for $J_s(nn)/J_b(nn) = 2.75$ and $13.4\ J_b(nn)/k_B$ for $J_s(nn)/J_b(nn) = 6.0$) are very close to these $T_{C,2d}$ values. As a more detailed look at the approach to this limiting behavior, we in Fig. 5 show $T_{C,surf}/T_{C,bulk}$ from our calculations and $T_{C,2d}/T_{C,bulk}$ from prior analytical treatments as a function of $J_s(nn)/J_b(nn)$ [16-18]. We find that, when $J_s(nn)/J_b(nn)$ is greater than about 3.0, $T_{C,surf}/T_{C,bulk}$ increases almost linearly with an increase in $J_s(nn)/J_b(nn)$ and is essentially identical to $T_{C,2d}/T_{C,bulk}$. Thus, for $J_s(nn)/J_b(nn)$ greater than this value, the exchange interactions between the surface and the second layer are expected to have negligible effects on the spin arrangements in the surface layer, and, as a result, the behavior at the surface should be rather close to that of a purely two-dimensional Ising ferromagnetic lattice.

We next consider in more detail the case of a strongly enhanced surface interaction with $J_s(nn)/J_b(nn) = 6.0$, and show the intra-layer spin-spin correlation functions in each layer (Fig. 6(a)) and the inter-layer spin-spin correlation functions between pairs of adjacent layers (Fig. 6(b)). Also in Fig. 6(c), we show the overall spin-spin correlation function, again for $J_s(nn)/J_b(nn) = 6.0$; here, each layer has been averaged with equal weight, although photoemission and other electron capture or emission experiments will tend to much more strongly weigh the near-surface layers. The spin-spin correlation curve corresponding to the surface layer in Fig. 6(a) has a significantly higher transition temperature of $T_{C,surf}/T_{C,bulk} \approx 3.0$, as compared to the curves for the other layers which have almost the same transition temperature as the bulk. All of the inter-layer spin-spin correlation curves (Fig. 6(b)) show similar features and drop off suddenly around the bulk Curie temperature $T_{C,bulk}$ ($\approx 4.5\ J_b(nn)/k_B$). The overall spin-spin correlation curve in Fig. 6(c) has a step-like falloff around $T_{C,bulk}$, then decreases smoothly with increasing in temperature until around $T_{C,surf}$, where another step-like falloff appears. For temperatures above $T_{C,surf}$, the spin-spin correlation function decreases slowly to zero. Overall, there are thus only two distinct transitions in these spin-spin correlation curves, one very close to the bulk critical temperature $T_{C,bulk}$ and the other at a much higher temperature $T_{C,surf}$ due to surface-enhanced interactions. There is no evidence of any intermediate step-like features or significant broadening due to intermediate transition temperatures for sub-surface layers.

By flipping spins on one sublattice, it is easily seen that the Hamiltonians of ferromagnetic and antiferromagnetic systems are equivalent to each other in the simple cubic Ising model with nn interactions only.

Thus, the above results for a ferromagnetic Ising lattice would be the same as those for an antiferromagnetic Ising lattice except that the spin-spin correlation functions between nearest neighbors(nn) would have opposite sign, and $T_{C,bulk}$ and $T_{C,surf}$ would be replaced by $T_{N,bulk}$ (bulk Néel temperature) and $T_{N,surf}$ (surface Néel temperature) respectively.

Thus considering these results as representative also of an antiferromagnetic surface without frustration, we note that the curve in Fig. 6(c) is at least qualitatively similar to the experimental SPPD data for MnO in Fig. 1: in both cases, there are two distinct transitions, one at around $T_{N,bulk}$ and the other at what can now be termed $T_{N,surf}$ which can be much higher than $T_{N,bulk}$ if $J_s(nn)/J_b(nn)$ is large enough. However, our calculated spin-spin correlation functions show no evidence of a high temperature transition that is limited to SRMO, and in fact none is expected within this model. Thus, it is possible that the high-temperature transitions seen in SPPD are surface-specific transitions, with the high surface sensitivity of the experiment leading to a greater emphasis of the surface transition.

III.2 Frustrated Antiferromagnetic Ising Lattices with nn and nnn Interactions

We now consider a more realistic model of the near-surface behavior in an antiferromagnetic lattice such as $KMnF_3$ and MnO in which spin frustration is included via next-nearest-neighbor interactions, as already introduced in Eq. 2. In estimating the relative strengths of the nn and nnn interactions, we make use of prior experimental data for some similar systems. For example, by studying the spin-wave dispersion curves of antiferromagnetic $KMnF_3$ [19, 20] and $RbMnF_3$ [20, 21] at 4.2 K by means of neutron inelastic scattering, it has been found that the next-nearest-neighbor exchange interaction J(nnn) is much smaller than the nearest-neighbor exchange interaction J(nn). For $KMnF_3$, $J(nn)/k_B = -3.8 \pm 0.04$ K and $J(nnn)/k_B = 0.11 \pm 0.02$ K; For $RbMnF_3$, $J(nn)/k_B = -3.4 \pm 0.3$ K and $J(nnn)/k_B = 0.0 \pm 0.2$ K. Thus, to begin this discussion, the exchange interaction between next-nearest neighbors J(nnn) has been arbitrarily, but plausibly, set to 0.1 times the corresponding value for nearest neighbors: $J(nnn) = 0.1 \cdot J(nn)$, and the signs of both have been reversed compared to the ferromagnetic case of the last section. Later in this paper, we investigate various J(nnn)/J(nn) values for completeness.

In Fig. 7. the spin-spin correlation functions for different surface exchange strengths $J_s(nn)/J_b(nn)$ = 1.00, 1.90, 2.75, 4.35, and 6.00 are compared with the corresponding ones calculated for a frustrated bulk system with $J_b(nn) = -1.0$ and $J_b(nnn) = 0.1\ J_b(nn)$. The intra-layer spin-spin correlation functions in the surface layer are shown in Fig. 7(a) and the inter-layer spin-spin corelations functions between the surface and the 2^{nd} layer are shown in Fig. 7(b). Fig. 7(c) shows the spin-spin correlation functions in the 2^{nd} layer. This figure is thus the antiferromagnetic analogue of Fig. 4, and both the intra-layer and inter-layer spin-spin correlation functions are very similar to those in Fig. 4, except for a trivial change in sign. For these choices of parameters, as in the case of ferromagnetic systems, there is no indication of transition temperatures significantly different from $T_{N,bulk}$ in the 2^{nd} to 5^{th} layers. Again in parallel with the ferromagnetic case, the temperature $T_{N,surf}$ for the step-like falloff of the surface intra-layer spin-spin correlation functions increases rapidly with an increase in exchange interactions (Fig. 7(a)). When $J_s(nn)/J_b(nn) = 2.75$, $T_{N,surf}/T_{N,bulk}$ is about 1.8, but when $J_s(nn)/J_b(nn)$ is increased to 6.0, $T_{N,surf}/T_{N,bulk}$ is increased to about 3.9. The inter-layer spin-spin correlations between the surface and the second layer and the intra-layer spin-spin correlations in the 2^{nd} layer (Figs. 7(b) and 7(c)) are affected very little by the change in surface exchange interactions. This again indicates that the surface layer can exhibit magnetic behavior very different from that of the bulk, and rather close to the corresponding two-dimensional case.

In Fig. 8, we show $T_{N,surf}/T_{N,bulk}$ as a function of $J_s(nn)/J_b(nn)$, together with the corresponding curve of $T_{C,surf}/T_{C,bulk}$ from the ferromagnetic case in the prior section for comparison. We find that $T_{N,surf}/T_{N,bulk}$, like $T_{C,surf}/T_{C,bulk}$ for non-frustrated systems, increases almost linearly with $J_s(nn)/J_b(nn)$ when $J_s(nn)/J_b(nn)$ is greater than about 3.0. As in ferromagnetic systems, this indicates that the magnetic behavior at the surface is close to that of purely two-dimensional case. However, $T_{N,surf}/T_{N,bulk}$ increases more rapidly than $T_{C,surf}/T_{C,bulk}$ with $J_s(nn)/J_b(nn)$. This is found to be due to the fact that frustration lowers the bulk critical temperature more than that in the surface layer at this case. That is, there is a higher degree of frustration in the bulk than in the surface for a fixed $J(nnn)/J(nn)$, since the ratio of nnn to nn coordination numbers (N(nnn)/N(nn)) is higher in the bulk: $N_{bulk}(nnn)/N_{bulk}(nn) = 12/6$ and $N_{surf}(nnn)/N_{surf}(nn) = 8/5$.

In Fig. 9 we show for this antiferromagnetic case the intra-layer spin-spin correlation functions between nearest neighbors (9(a)) and next-nearest neighbors (9(b)) for $J_s(nn)/J_b(nn) = 6.0$ and again $J(nnn) = 0.1 \cdot J(nn)$. Also in Fig. 9(c) we show the overall value of spin-spin correlation functions between nearest neighbors for the first five layers near the surface, with each layer again treated with equal weight. (This is thus similar to Fig. 6(c) for the ferromagnetic case, but with next-nearest neighbors now included). The spin-spin correlation functions show similar features for both the nn and nnn cases. The intra-layer spin-spin correlation curves at the surface have a significantly larger transition temperature compared with the curves of the other layers, with the latter having almost the same transition temperature as the bulk for both the nn and nnn cases. The overall spin-spin correlation curve in Fig. 9(c) has a step-like feature around $T_{N,bulk}$, then increases smoothly with increasing in temperature until around $T_{N,surf}$, where another step-like feature appears. At temperatures higher than $T_{N,surf}$, the spin-spin correlation function increases slowly to zero. Thus, in frustrated antiferromagnetic systems, the overall spin-spin correlation function still shows the same trends as the SPPD experimental data in Fig. 1(a), and these results give no indication of a higher temperature transition that is unique to SRMO. This further suggests that the high-temperature transitions observed in both $KMnF_3$ and MnO could be due to surface-specific phenomenon.

We have also studied the behavior of spin-spin correlation functions on and near the surfaces of antiferromagnetic systems for various J(nnn)/J(nn) values ranging from -0.25 to 0.35 and with $J_s(nn)/J_b(nn)$ = 3.0 and 6.0 respectively. In general, we find that frustration does not have major effects on the general behavior of the spin-spin correlation functions. For example, the magnetic behavior at the surface is rather unique and very little affected by the other layers, like the results we have shown before for the J(nnn)/J(nn) = 0 and 0.1 cases. The various spin-spin correlation functions exhibit distinct step-like features at only two temperatures, one of which is due to the bulk transition and the other to the surface transition.

In Fig. 10, we summarize this behavior by showing $T_{N,surf}$, $T_{N,bulk}$ and $T_{N,surf}/T_{N,bulk}$ as a function of J(nnn)/J(nn) for the two cases $J_s(nn)/J_b(nn)$ = 3.0 and 6.0. In Fig. 10(a), we show that $T_{N,surf}$ decreases monotonically as J(nnn)/J(nn) increases from -0.25 to 0.35, as expected due to the concomitant increase in frustration. However, $T_{N,bulk}$ behaves differently as a function of J(nnn)/J(nn): it decreases monotonically as J(nnn)/J(nn) increases from -0.25 to 0.25 and reaches its minimum (about 1.1 $J_b(nn)/k_B$) at J(nnn)/J(nn) = 0.25. Then, it increases monotonically to about 1.7 $J_b(nn)/k_B$ as J(nnn)/J(nn) increases from 0.25 to 0.35. This phenomenon is caused by the switching of the bulk antiferromagnetic spin configurations of simple cubic frustrated antiferromagnetic lattices at J(nnn)/J(nn) = 0.25. For example, in Fig. 11 we show two possible ground-state spin configurations on simple cubic antiferromagnetic lattices with nn and nnn interactions. According to the Hamiltonian in the bulk:

$$H = -J_b(nn)\Sigma_{nn,bulk}S_iS_j - J_b(nnn)\Sigma_{nnn,bulk}S_iS_j \qquad (3)$$

we can get that for the spin configuration in Fig. 11(a) the ground-state energy

$$U_a = J_b(nn)\ \{6 - 12\ J_b(nnn)/J_b(nn)\} \qquad (3a)$$

and for the spin configuration in Fig. 11(b) the ground-state energy

$$U_b = J_b(nn)\ \{2 + 4\ J_b(nnn)/J_b(nn)\}. \qquad (3b)$$

By comparing U_a with U_b, we find that the ground-state energy $U_a <$ the ground-state energy U_b if $J_b(nnn)/J_b(nn) < 0.25$, $U_a = U_b$ when $J_b(nnn)/J_b(nn) = 0.25$ and $U_a > U_b$ if $J_b(nnn)/J_b(nn) > 0.25$ since $J_b(nn)$ is negative for antiferromagnetic lattices. Thus, when $J_b(nnn)/J_b(nn) < 0.25$, the lattices studied here prefer the antiferromagnetic spin configuration shown in Fig. 11(a). This spin configuration will switch to the one shown in Fig. 11(b) when $J_b(nnn)/J_b(nn) > 0.25$ because in this case the spin configuration in Fig. 11(b) has lower internal energy than in Fig. 11(a). From equations (3a) and (3b), we can also see that U_a increases as $J_b(nnn)/J_b(nn)$ increases, while U_b decreases as $J_b(nnn)/J_b(nn)$ increases, and the internal energy reaches its maximum at $J_b(nnn)/J_b(nn) = 0.25$ where $U_a = U_b$. Since the Neel temperature is related to the net statistically-averaged interactions of neighboring spins on a given spin, it is expected that the bulk Neel temperature decreases when $J_b(nnn)/J_b(nn)$ increases from -0.25 to 0.25, reaches a minimum at $J_b(nnn)/J_b(nn) = 0.25$, then increases with increasing in $J_b(nnn)/J_b(nn)$ from 0.25 to 0.35, as shown in Fig. 10(a). The antiferromagnetic spin configuration switching phenomenon has also been observed by Landau and Binder [22], Selke and Fisher [23] for simple square antiferromagnetic lattices at $J(nnn)/J(nn) = 0.5$. These two spin configurations differ in their ordering wavevector. The magnetic structure factor of the spin configuration in Fig. 11(a) would exhibit a peak at k = (pi, pi, pi), while in Fig. 11(b) would have a peak at (pi, pi, 0).

In Fig. 10(b), we also show $T_{N,surf}/T_{N,bulk}$ as a function of $J(nnn)/J(nn)$: This quantity increases monotonically as $J(nnn)/J(nn)$ increases from -0.25 to 0.25 and reaches a sharp maximum (about 3.6 for $J_s(nn)/J_b(nn) = 3.0$ and 7.3 for $J_s(nn)/J_b(nn) = 6.0$) when $J(nnn)/J(nn)$ is about 0.25. Then, $T_{N,surf}/T_{N,bulk}$ decreases to about 1.9 for $J_s(nn)/J_b(nn) = 3.0$ and 3.8 $J_s(nn)/J_b(nn) = 6.0$ as $J(nnn)/J(nn)$ increases from 0.25 to 0.35. Also, over the full range of $J(nnn)/J(nn)$ values, $T_{N,surf}/T_{N,bulk}$ at $J_s(nn)/J_b(nn) = 6.0$ is about twice of that at $J_s(nn)/J_b(nn) = 3.0$, indicating that the surface magnetic order depends primarily on $J_s(nn)$ and further showing that the surface order behaves almostly independently from the bulk.

Finally, we consider the behavior of the Curie-Weiss constant at the surface (Θ_{surf}) with respect to that in the bulk (Θ_{bulk}) for antiferromagnetic lattices studied above for comparison. Based on mean-field theory, the Curie-Weiss constant should represent a sum over all nn and nnn interactions [24]. Also, prior SPPD results have suggested that there might be a connection between Θ_{bulk} and the high-temperature transition temperature [6,8]. We have therefore calculated $\Theta_{surf}/\Theta_{bulk}$ as a function of $J_s(nn)/J_b(nn)$ and $J(nnn)/J(nn)$, as shown in Fig. 12(a) and 12(b) respectively. In Fig. 12(a), the value of $\Theta_{surf}/\Theta_{bulk}$ shows the expected linear increase with an increase in $J_s(nn)/J_b(nn)$. For the case of $J(nnn)/J(nn) = 0.1$, the value of $\Theta_{surf}/\Theta_{bulk}$ is about 1.9 when $J_s(nn)/J_b(nn) = 2.75$ and about 3.9 when $J_s(nn)/J_b(nn) = 6.0$. These values are close to the corresponding $T_{N,surf}/T_{N,bulk}$ values (about 1.8 for $J_s(nn)/J_b(nn) = 2.75$ and about 3.9 for $J_s(nn)/J_b(nn) = 6.0$). However, in Fig. 12(b), we show that $\Theta_{surf}/\Theta_{bulk}$ decreases monotonically with an increase in $J(nnn)/J(nn)$. This is expected due to the fact that the sum over nn and nnn interactions increases faster in the bulk than in the surface layer as $J(nnn)/J(nn)$ increases because of the higher ratio of coordination numbers of nnn to nn in the bulk than in the surface (i.e. Θ_{bulk} increases faster than Θ_{surf} as $J(nnn)/J(nn)$ increases). This is different from the behavior of $T_{N,surf}/T_{N,bulk}$ as a function of $J(nnn)/J(nn)$ shown in Fig. 10, and such a difference is understandable because the Neel temperature is related to the net statistically-averaged interactions of neighboring spins on a given spin while the Curie-Weiss constant is just the simple sum over all the neighboring interactions.

IV CONCLUSIONS

We have studied spin-spin correlation functions near both ferromagnetic and antiferromagnetic (frustrated and unfrustrated) surfaces as derived from Monte Carlo simulations on simple-cubic Ising lattices. The relative strengths of surface exchange interactions were modified in an attempt to model prior experiments in which magnetic transition temperatures higher than those of the bulk have been observed, with particular emphasis on spin-polarized photoelectron diffraction studies of antiferromagnets. For sufficient enhancement of the surface interactions, the overall spin-spin correlation function near the surface showed behavior that is qualitatively similar to what has been observed in experiment. Two distinct step-like features occurred for this function: one is around the bulk critical temperature $T_{N,bulk}$ (or for ferromagnets $T_{C,bulk}$), and the other is around the surface critical temperature $T_{N,surf}$ (or for ferromagnets $T_{C,surf}$). If the surface-to-bulk ratio of nearest-neighbor exchange interactions $J_s(nn)/J_b(nn)$ is high enough, $T_{N,surf}$ (or $T_{C,surf}$) can be well above $T_{N,bulk}$(or $T_{C,bulk}$), as observed experimentally. For $J_s(nn)/J_b(nn)$ greater than about 3.0, the magnetic behavior at the surface is found to be essentially two-dimensional and very little affected by the other layers. The abrupt step-like falloff of spin-spin correlation functions well above the bulk transition temperatures $T_{N,bulk}$ (or Curie temperature $T_{C,bulk}$) is due to the enhanced exchange interactions in the surface layer and gives rise to a surface-specific transition. All the other spin-spin correlation functions except that in the surface layer have similar behavior and an abrupt falloff around the bulk transition temperature $T_{N,bulk}$ (or $T_{C,bulk}$). The addition of frustration through antiferromagnetic next-nearest-neighbor interaction also does not have major effects on the general bahavior of the spin-spin correlation functions. Thus, this model does not predict a distinct high-temperature transition in short-range magnetic order (SRMO), although this has been proposed as one possible explanation for the prior SPPD results [4,5,6,8]. On the basis of these results and the fact that the experimental spin asymmetry in SPPD is directly linked to spin-spin correlation functions, we conclude that the falloff of the spin asymmetry well above the bulk critical temperature could be due to a surface-specific magnetic order transition. However, it will require more experimental data and a more quantitative knowledge of the actual coupling bulk and surface parameters for real systems to make this a definitive conclusion. The results presented here should also be useful in assessing the phenomenology of other surface-specific magnetic transitions.

Finaly, we note that, in real materials, a more appropriate model would be the Heisenberg Hamiltonian, unless some form of surface relaxation induces a high magnetic anisotropy. Pure Heisenberg systems cannot have a separate finite temperature surface transition, owing to the Mermin-Wagner theorem [25]. However, the correlation length of the two-dimensional Heisenberg model increases very rapidly as T is lowered. Thus it may be that surface spin order at moderate distances will appear at rather higher temperatures than the bulk temperature ($T_{C,bulk}$ for ferromagnets and $T_{N,bulk}$ for antiferromagnets), in a manner that is qualitatively similar to what we have observed here. The much greater computational complexity of the Heisenberg model has prevented our exploring it here, but this would certainly be of interest for future work.

This work is supported in part by the Department of Energy, Basic Energy Sciences, Materials Sciences Division, under Contract No. DE-AC03-76SF00098, and the Office of Naval Research under Contracts No. N00014-90-5-1457 and N00014-94-1-0162.

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FIGURE CAPTIONS:

Fig. 1: Mn 3s experimental spin asymmetries S_{expt} with Mo Mξ excitation are plotted as a function of temperature at a polar angle θ = 90^o (normal emission) and an azimuthal orientation of ϕ = 0° ([010]

azimuth). The temperature range covered is from ≈50 degrees below $T_{N,bulk}$ to ≈620 degrees above it (from ref. 8).

Fig. 2: Schematic illustration of the simple cubic lattice considered here with representative surface and bulk exchange interactions indicated.

Fig. 3: Temperature dependence of near-surface intra-layer and inter-layer spin-spin correlation functions between nearest neighbors (nn) for a ferromagnetic system with $J_s(nn)/J_b(nn) = 1.0$. (a) Intra-layer spin-spin correlation functions from the surface to the 5^{th} layer. (b) Inter-layer spin-spin correlation functions between different pairs of adjacent layers near the surface.

Fig. 4: Temperature dependence of intra-layer and inter-layer spin-spin correlation functions between nearest neighbors (nn) for different relative strengths of surface exchange: $J_s(nn)/J_b(nn)$ = 1.0, 1.90, 2.75, 4.35, and 6.0, and for a reference bulk case. (a) Intra-layer spin-spin correlation functions for the surface layer and for the bulk case; (b) As (a), but inter-layer spin-spin correlation functions between the surface and the second layer; (c) As (a), but in the second layer.

Fig. 5: The ratio of surface critical temperature $T_{C,surf}$(or $T_{N,surf}$) and two-dimensional critical temperature $T_{C,2d}$ to bulk critical temperature $T_{C,bulk}$ as a function of $J_s(nn)/J_b(nn)$.

Fig. 6: Temperature dependence of intra-layer and adjacent inter-layer spin-spin correlation functions between nearest neighbors for a ferromagnetic system with $J_s(nn)/J_b(nn) = 6.0$. (a) Intra-layer spin-spin correlation functions from the surface to the 5^{th} layer; (b) Inter-layer spin-spin correlation functions between different neighboring layers near the surface; (c) The overall spin-spin correlation function for the first five layers near the surface with equal weight.

Fig. 7: As Fig. 4, but for a frustrated antiferromagnetic, with the next-nearest neighbor interaction added as $J(nnn) = 0.1 \cdot J(nn)$.

Fig. 8: The ratio of surface critical temperature $T_{N,surf}$ to bulk critical temperature $T_{N,bulk}$ as a function of $J_s(nn)/J_b(nn)$ for a frustrated antiferromagnetic system with $J(nnn) = 0.1 \cdot J(nn)$. Also the corresponding ferromagnetic curve in Fig. 5 is presented here for comparison.

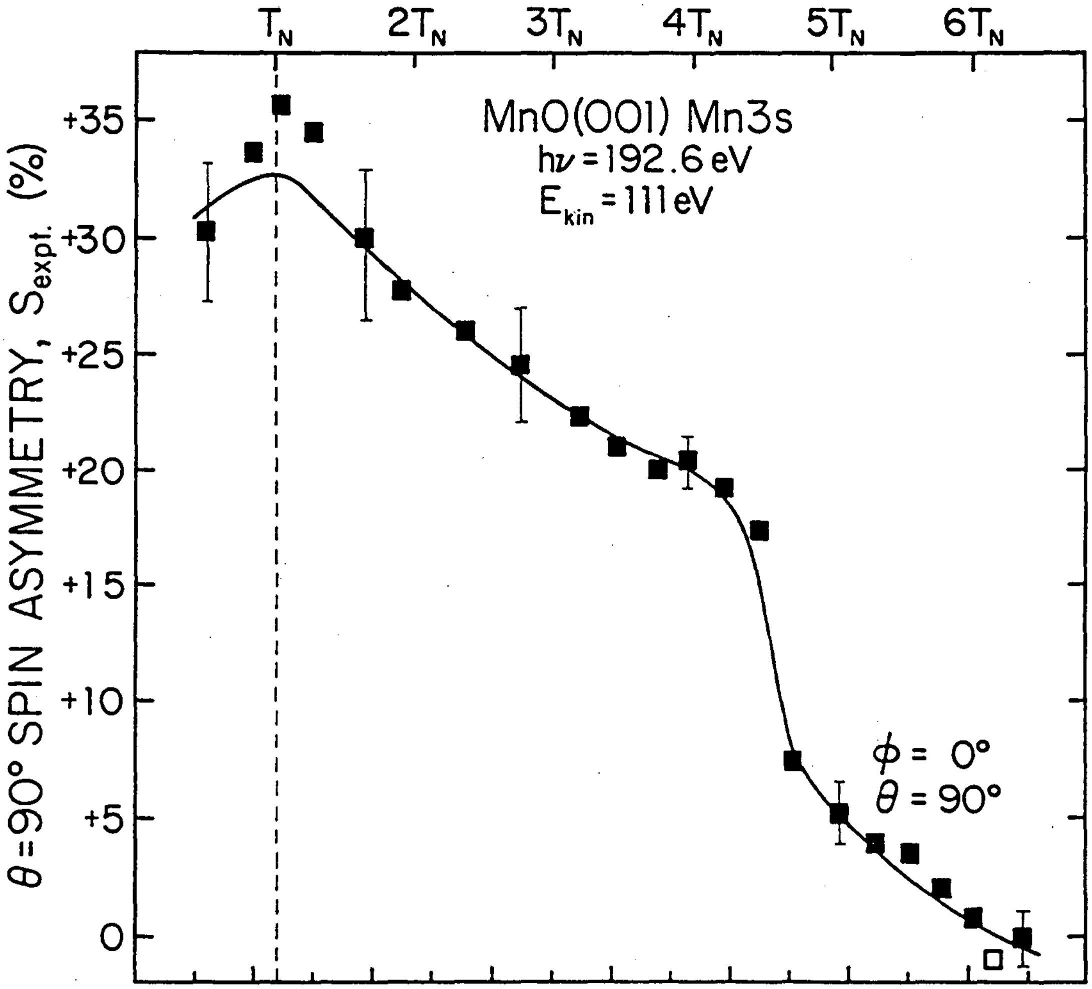
Fig. 9: (a),(b) Temperature dependence of intra-layer spin-spin correlation functions from the surface to the 5^{th} layer for a frustrated antiferromagnetic system with $J_s(nn)/J_b(nn) = 6.0$ and $J(nnn) = 0.1 \cdot J(nn)$. (a) Between nearest neighbors; (b) Between next-nearest neighbors. (c) The overall spin-spin correlation function for the first five layers near the surface with each layer getting equal weight.

Fig. 10: (a) Surface critical temperature $T_{N,surf}$ and bulk critical temperature $T_{N,bulk}$ as a function of $J(nnn)/J(nn)$ for antiferromagnetic

systems when $J_s(nn)/J_b(nn)$ = 3.0 and 6.0 respectively; (b) $T_{N,surf}/T_{N,bulk}$ as a function of J(nnn)/J(nn) when $J_s(nn)/J_b(nn)$ = 3.0 and 6.0 respectively as a result of (a).

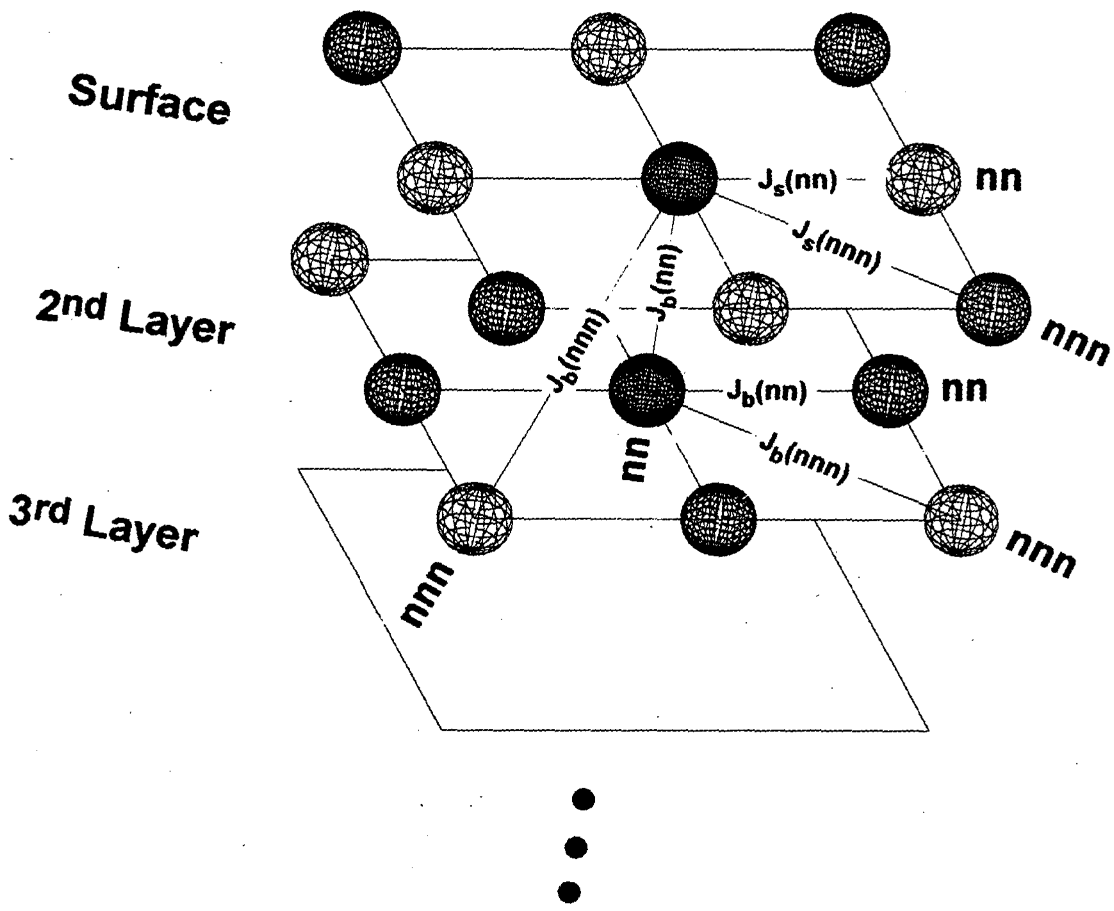
Fig. 11: Two possible antiferromagnetic spin configurations on simple cubic antiferromagnetic lattices with nn and nnn interactions.

Fig. 12: (a) The ratio of surface Curie-Weiss constant Θ_{surf} to bulk Curie-Weiss constant Θ_{bulk} as a function of $J_s(nn)/J_b(nn)$ when J(nnn)/J(nn) = 0.0 and 0.1 respectively. (b) The same ratio, but as a function of J(nnn)/J(nn) with $J_s(nn)/J_b(nn)$ = 3.0 and 6.0 respectively.



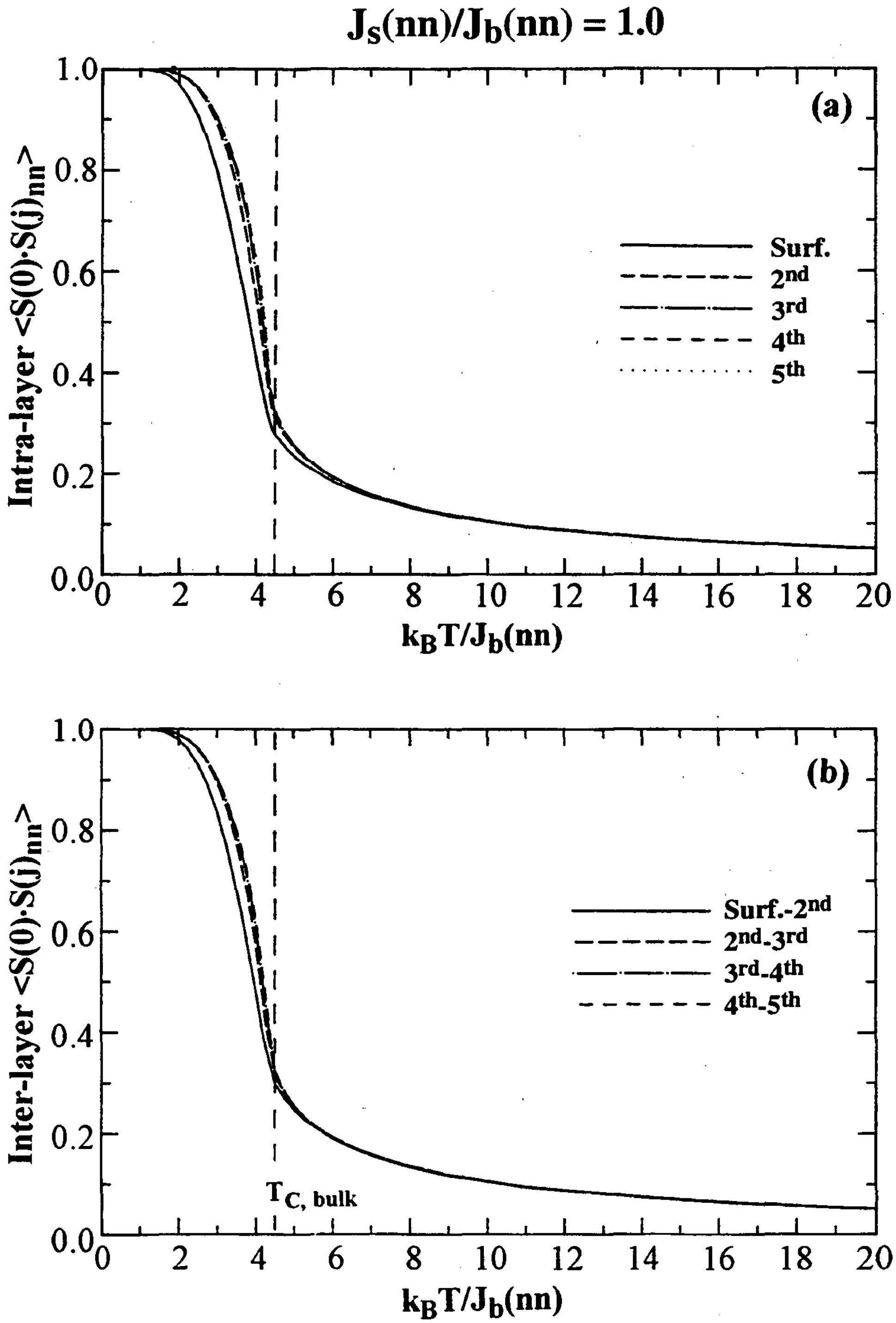
T_N
$2T_N$
$3T_N$
$4T_N$
$5T_N$
$6T_N$
MnO(001) Mn3s
$h\nu = 192.6$ eV
$E_{kin} = 111$ eV
$\phi = 0°$
$\theta = 90°$
$\theta = 90°$ SPIN ASYMMETRY, $S_{expt.}$ (%)
+35
+30
+25
+20
+15
+10
+5
0
0
100
200
300
400
500
600
700
TEMPERATURE (K)

Figure 1



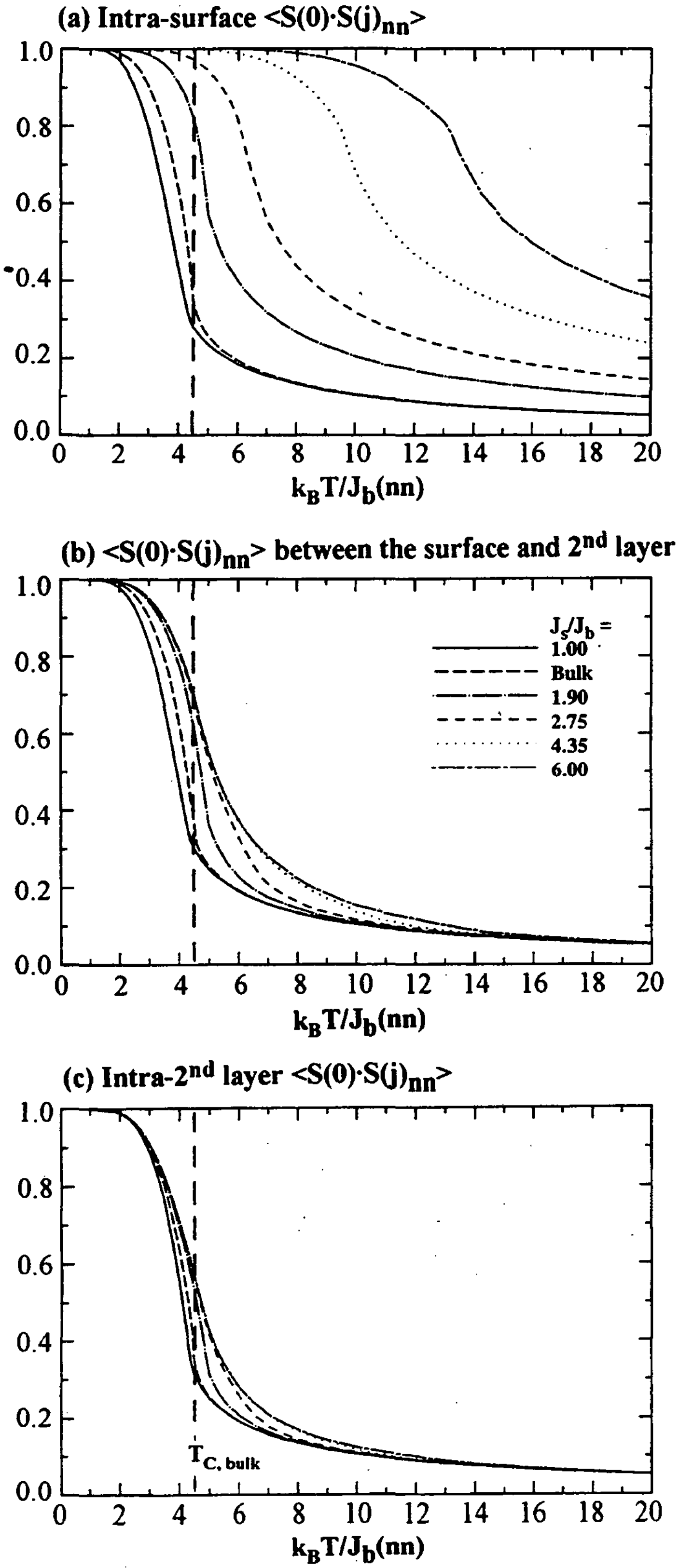
Surface
2nd Layer
3rd Layer
J_s(nn)
nn
J_s(nnn)
J_b(nn)
J_b(nnn)
nnn
J_b(nn)
nn
nn
J_b(nnn)
nnn
nnn

Figure 2



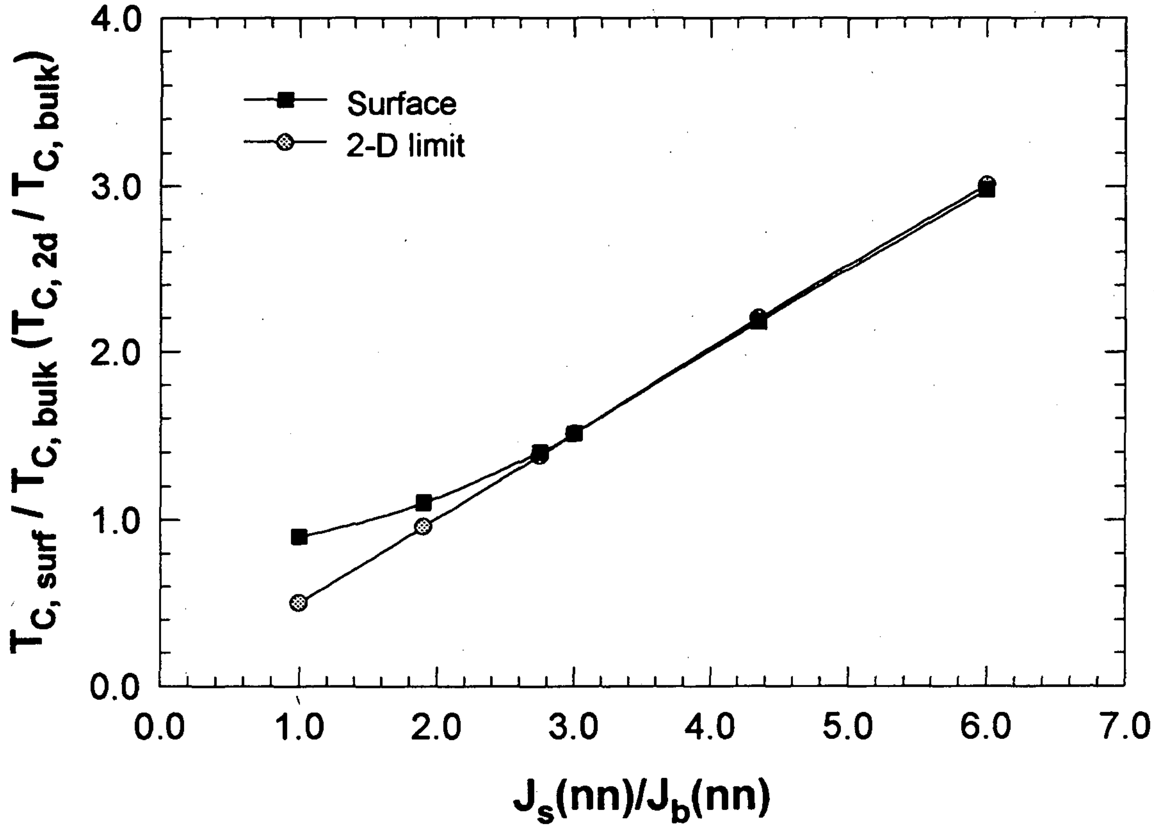
$J_s(nn)/J_b(nn) = 1.0$
(a)
Intra-layer $<S(0)\cdot S(j)_{nn}>$
Surf.
2nd
3rd
4th
5th
$k_BT/J_b(nn)$
(b)
Inter-layer $<S(0)\cdot S(j)_{nn}>$
Surf.-2nd
2nd-3rd
3rd-4th
4th-5th
$T_{C,\ bulk}$
$k_BT/J_b(nn)$

Figure 3



(a) Intra-surface <S(0)·S(j)nn>
(b) <S(0)·S(j)nn> between the surface and 2nd layer
(c) Intra-2nd layer <S(0)·S(j)nn>
1.0
0.8
0.6
0.4
0.2
0.0
0 2 4 6 8 10 12 14 16 18 20
kBT/Jb(nn)
Js/Jb =
1.00
Bulk
1.90
2.75
4.35
6.00
TC, bulk

Figure 4



Surface
2-D limit
$T_{C,\,surf} / T_{C,\,bulk}$ ($T_{C,\,2d} / T_{C,\,bulk}$)
$J_s(nn)/J_b(nn)$
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0

Figure 5

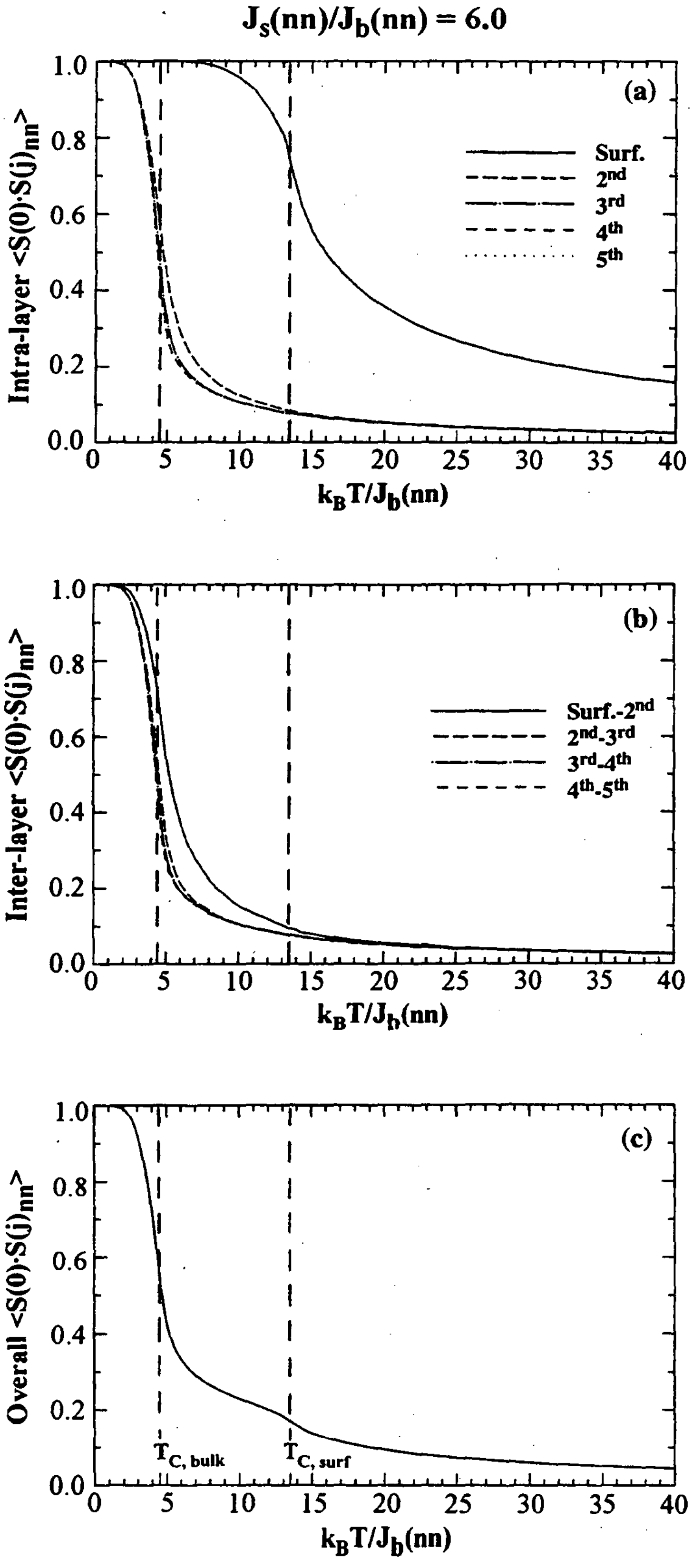
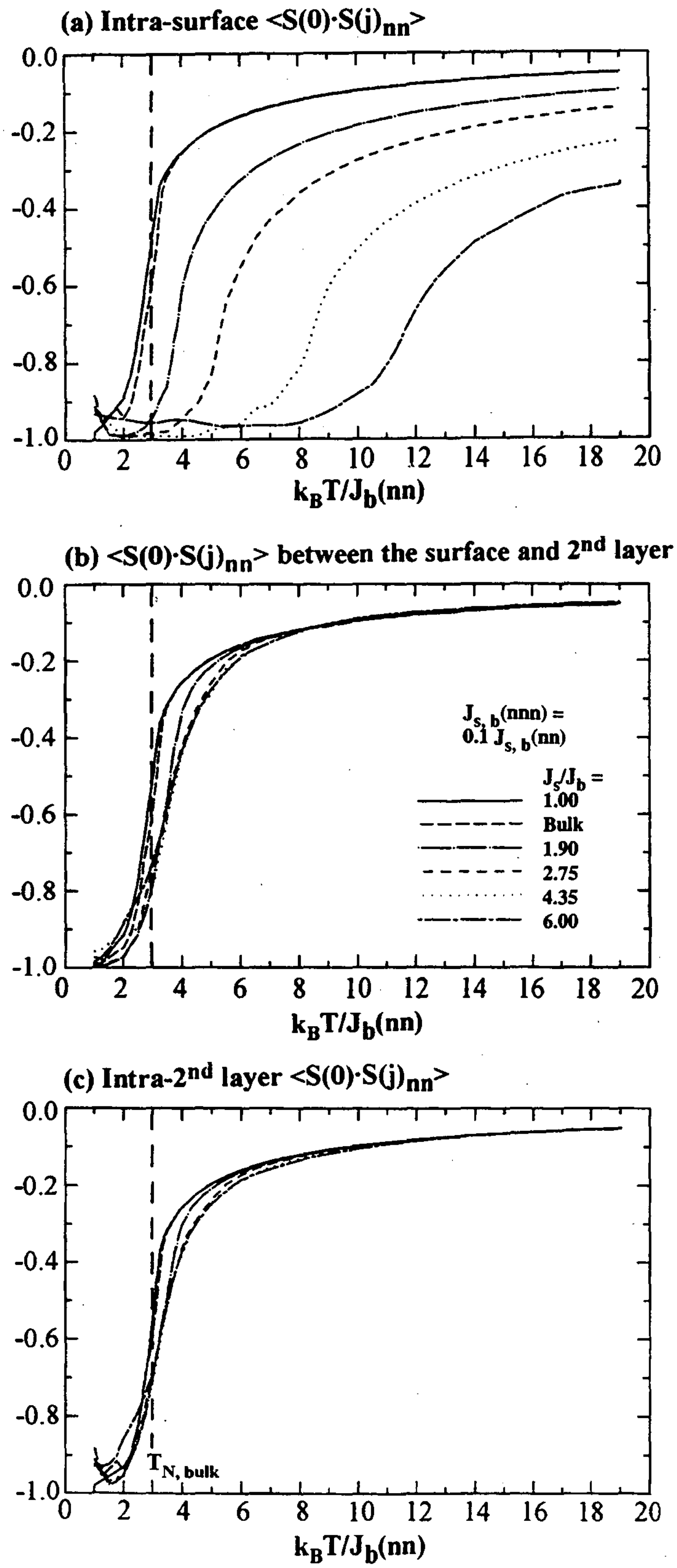
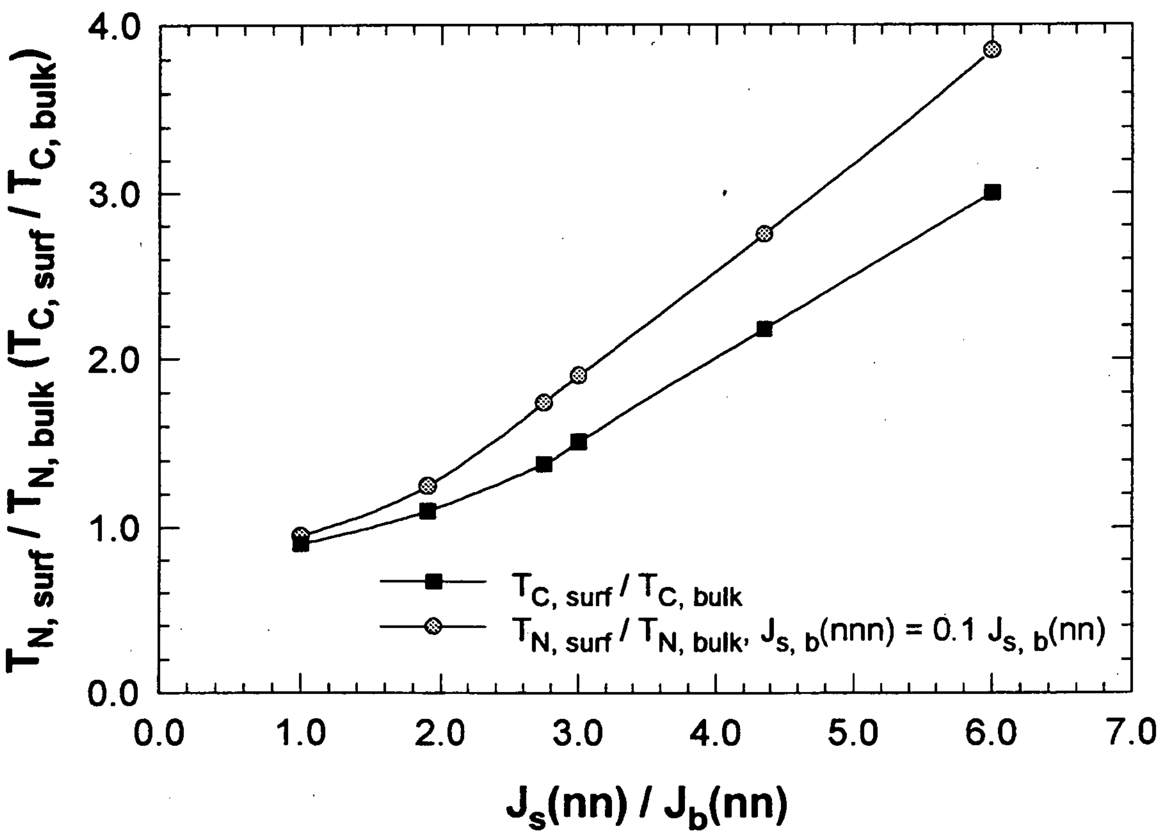

$J_s(nn)/J_b(nn) = 6.0$
(a)
Intra-layer $<S(0) \cdot S(j)_{nn}>$
Surf.
2nd
3rd
4th
5th
$k_B T/J_b(nn)$
(b)
Inter-layer $<S(0) \cdot S(j)_{nn}>$
Surf.-2nd
2nd-3rd
3rd-4th
4th-5th
$k_B T/J_b(nn)$
(c)
Overall $<S(0) \cdot S(j)_{nn}>$
$T_{C, bulk}$
$T_{C, surf}$
$k_B T/J_b(nn)$

Figure 6



(a) Intra-surface <S(0)·S(j)nn>
(b) <S(0)·S(j)nn> between the surface and 2nd layer
(c) Intra-2nd layer <S(0)·S(j)nn>
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
0 2 4 6 8 10 12 14 16 18 20
kBT/Jb(nn)
Js, b(nnn) = 0.1 Js, b(nn)
Js/Jb =
1.00
Bulk
1.90
2.75
4.35
6.00
TN, bulk

Figure 7



4.0
3.0
2.0
1.0
0.0
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
T_N, surf / T_N, bulk (T_C, surf / T_C, bulk)
J_s(nn) / J_b(nn)
T_C, surf / T_C, bulk
T_N, surf / T_N, bulk, J_s, b(nnn) = 0.1 J_s, b(nn)

Figure 8

$J_s(nn)/J_b(nn) = 6.0;\ J_{s,b}(nnn) = 0.1\ J_{s,b}(nn)$

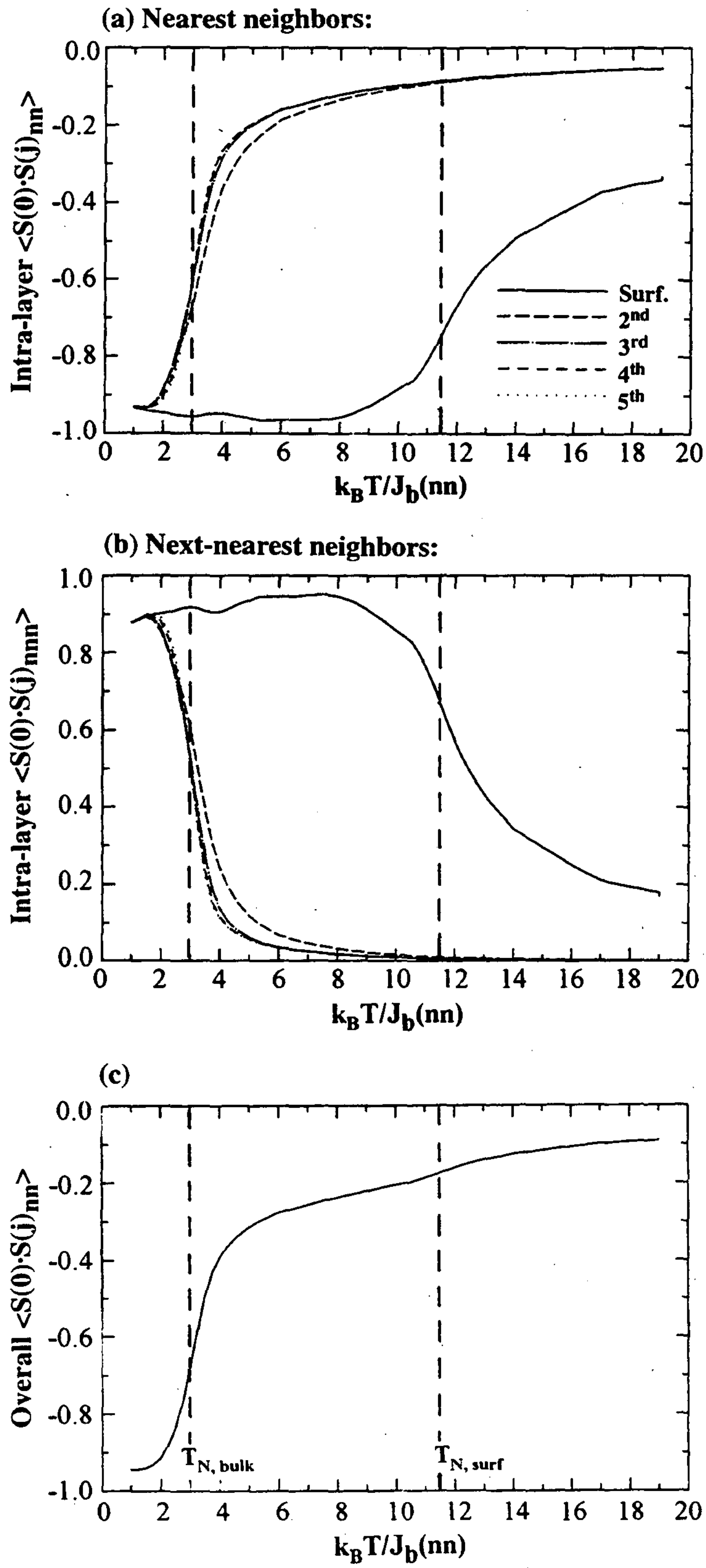


Figure 9

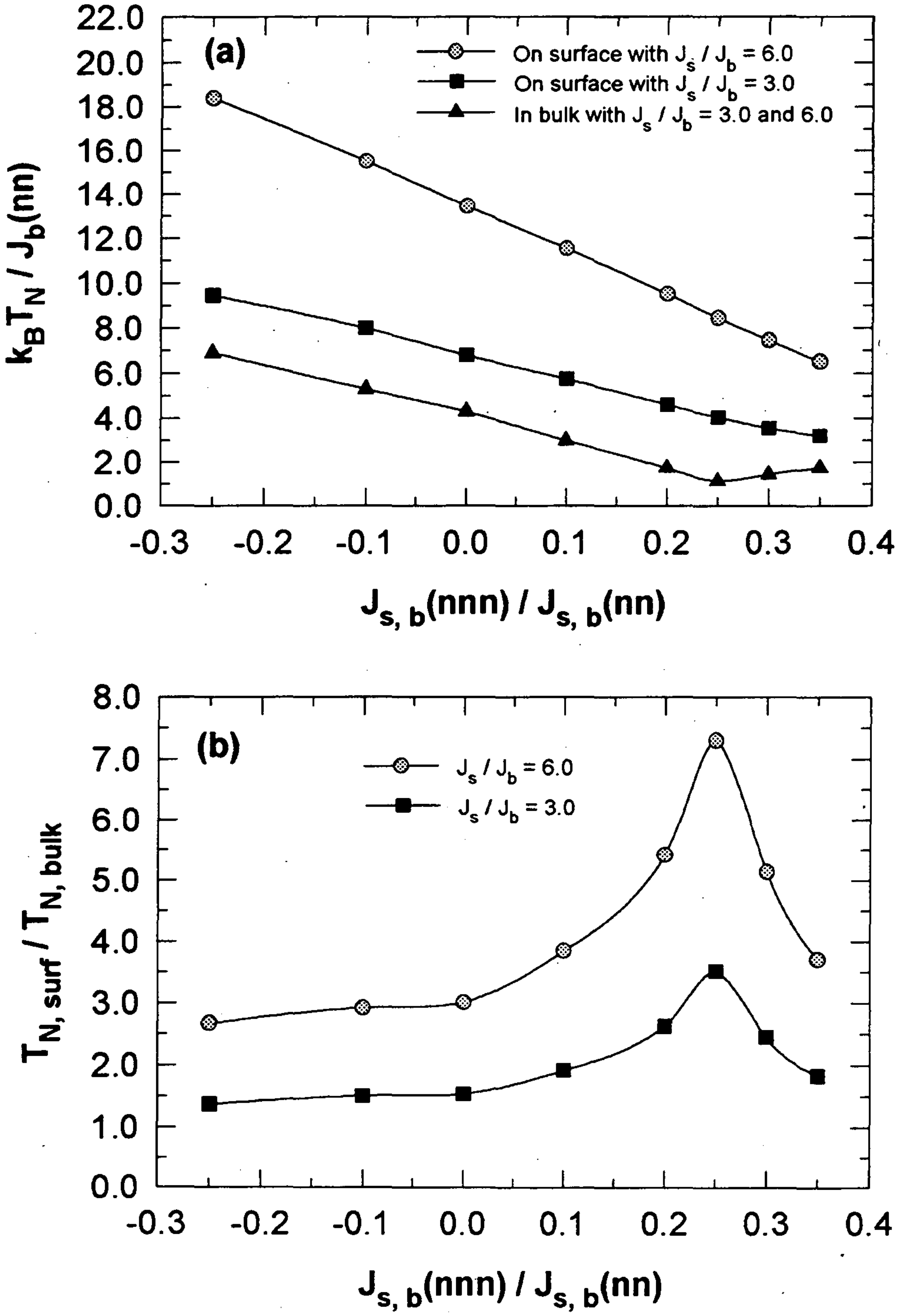

(a)
On surface with $J_s / J_b = 6.0$
On surface with $J_s / J_b = 3.0$
In bulk with $J_s / J_b = 3.0$ and 6.0
$k_B T_N / J_b(nn)$
$J_{s,b}(nnn) / J_{s,b}(nn)$
(b)
$J_s / J_b = 6.0$
$J_s / J_b = 3.0$
$T_{N,surf} / T_{N,bulk}$
$J_{s,b}(nnn) / J_{s,b}(nn)$

Figure 10

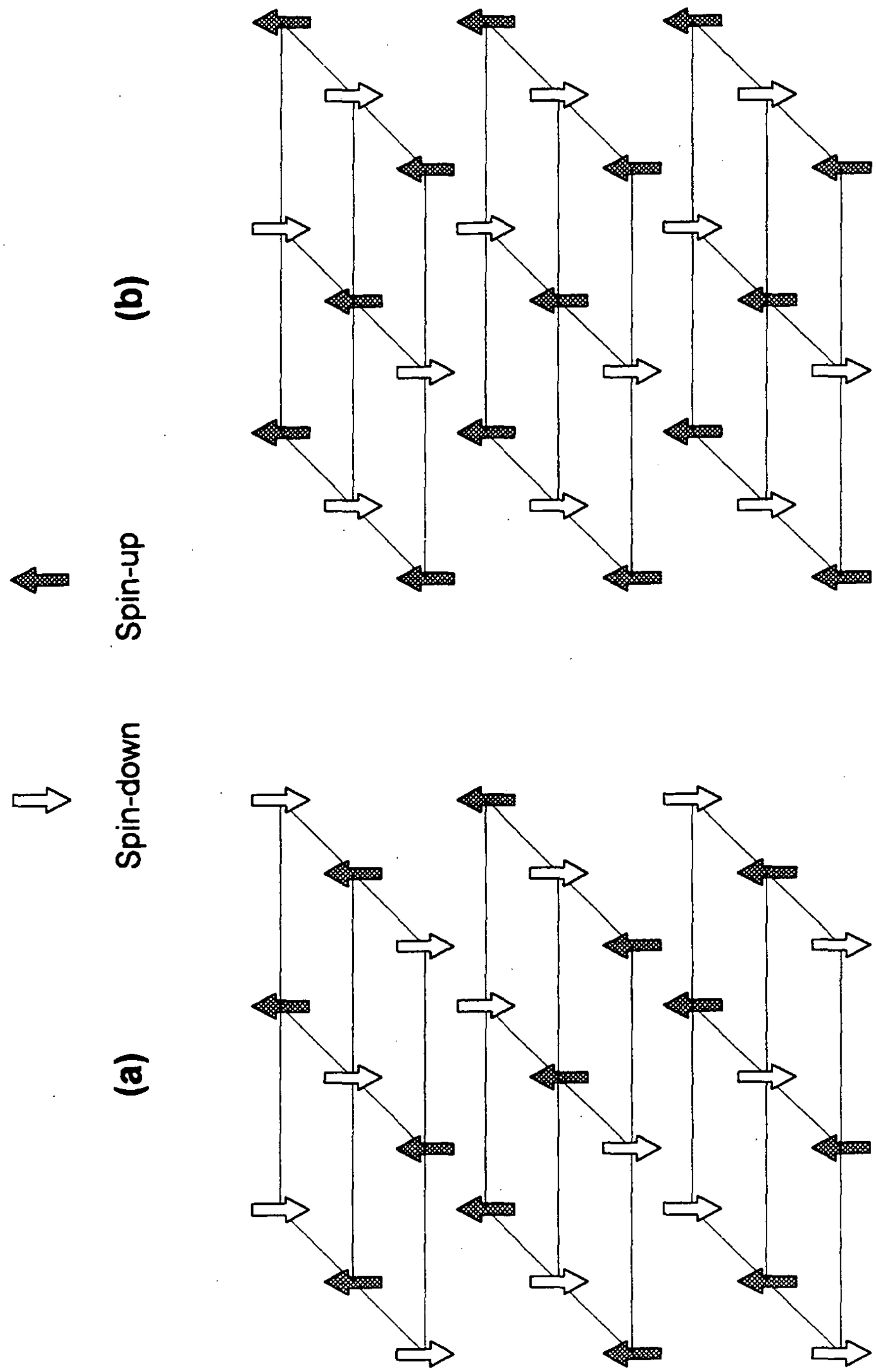


Figure 11

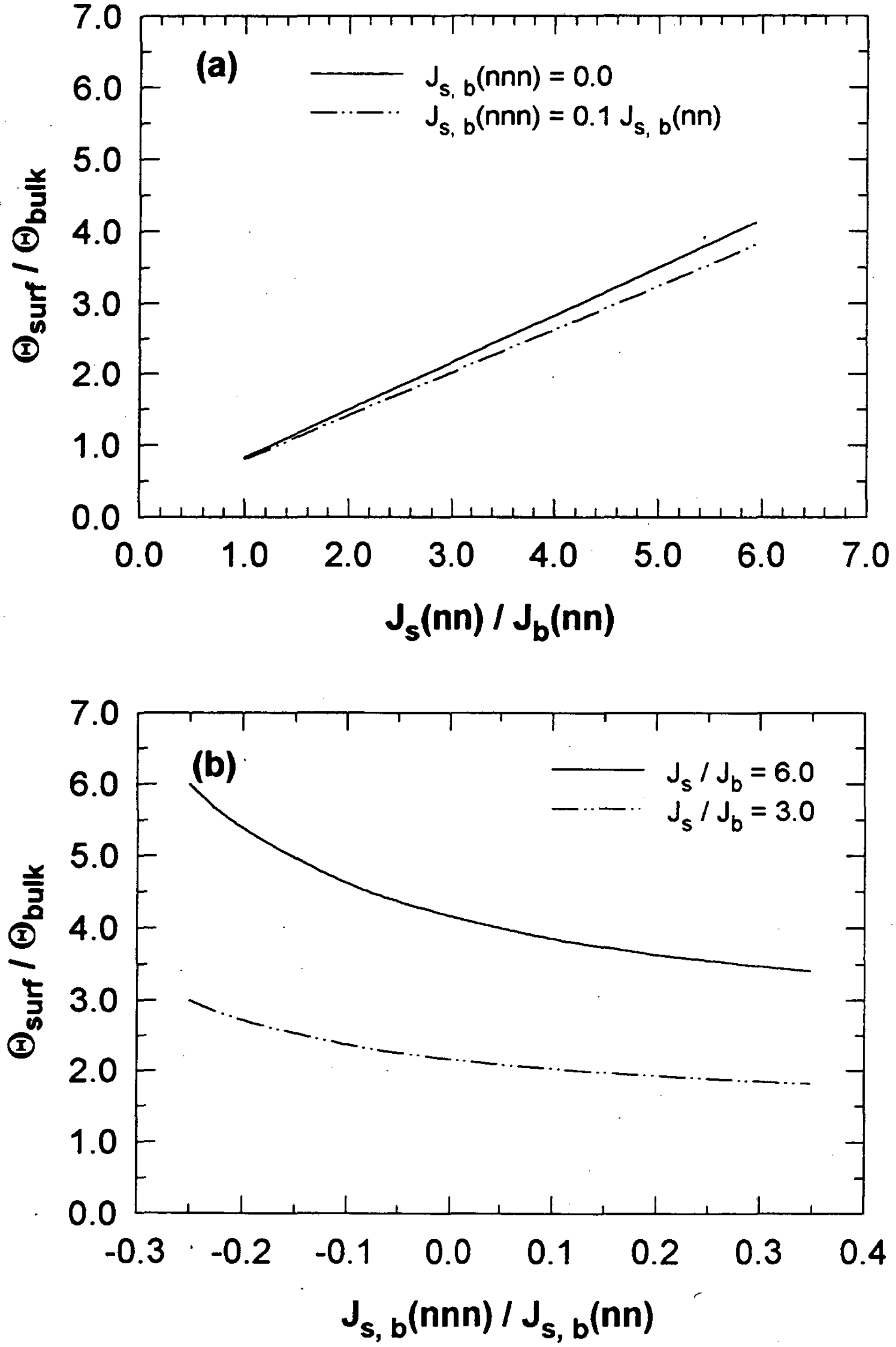

(a)
Js, b(nnn) = 0.0
Js, b(nnn) = 0.1 Js, b(nn)
Θsurf / Θbulk
Js(nn) / Jb(nn)
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
(b)
Js / Jb = 6.0
Js / Jb = 3.0
Js, b(nnn) / Js, b(nn)
-0.3
-0.2
-0.1
0.1
0.2
0.3
0.4

Figure 12

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