Simulation of ^{3}He crystal shapes

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Experimental results indicating roughening transitions in bcc ^{3}He (100), (110), and (211) facets were recently obtained by Wagner *et al.* We built computer models for these facets using a Lennard-Jones potential, including higher-nearest-neighbor interactions. By Monte Carlo simulations we obtained the transition temperatures of these facets; these fit the experimental limits quite well. [S0163-1829(97)01023-0]

In a recent letter, Wagner *et al.*,[1] described observations of facets on bcc ^{3}He crystals in the (110), (100), and (211) orientations, both in growth and in equilibrium for temperatures below 2.5 mK. The (110) facet had previously been observed at temperatures below 100 mK by Rolley, Balibar, and Gallet.[3]

Since helium crystals have been considered a good testing ground for theories of equilibrium surface roughening, Wagner *et al.*[1] discussed the relationship between the experimental results and a simple relationship arising from the Kosterlitz-Thouless (KT) theory.[4] This relates the roughening temperature of a facet to the surface stiffness and lattice-plane spacing in that orientation. However, it has been observed[5] that this relationship did not agree very well with the measurements made on ^{4}He; in particular, it suggested that the (1010) facet of ^{4}He should roughen at a higher temperature than (0001), in contradiction to experiment.

In this paper, we shall discuss the results in the light of simulations of crystal surfaces which we have been carrying out in order to understand the roughening temperatures of both ^{3}He and ^{4}He crystals. We shall show that for ^{3}He our numerical results also satisfy the relationship of the KT theory and agree with all the experimental data.

The roughening transition (RT) was proposed by Burton, Cabrera, and Frank, based on an analogy with the phase transition of a two-dimensional (2D) Ising model. Since that time, many more sophisticated models for the RT have been conceived, including the lattice-gas models and the solid-on-solid (SOS) models. Most published simulations have been made for lattice gas or SOS models on simple cubic systems (which correspond to no real materials). An important step forward was made by van Beijeren[2] who built an exactly solvable SOS model for a bcc (110) facet with nearest-neighbor interactions. But apart from this example, all other theoretical calculations of roughening involve either a renormalization group or other approximations or simulations.

Using the simplest understanding of roughening of helium crystals as a two-dimensional Ising transition on the exposed crystal facet[6,7] it is clear that, in the absence of higher-neighbor interactions, the only transitions expected at nonzero temperatures are on the **c** or (0001), **a** or (1010), and **s** or (1011) in ^{4}He and on the (110) facet in ^{3}He. These have all been discovered at relatively high temperatures. Touzani and Wortis (TW) (Ref. 7) first built two-dimensional (2D) Ising models for the three hcp facets of ^{4}He. Since the **a** and **s** facets contains atoms which are not exactly coplanar (having a different number of up and down neighbors), they adopted a technique of ''staggered magnetic field.'' In this technique, an energy penalty is paid by out-of-plane atoms in proportion to their number of nearest neighbors in the three-dimensional crystal. Since the analogy is to a spin system, this is described by a magnetic field which changes sign at the interface. TW found good agreement between their calculated roughening temperatures and those found in experiment for ratios between the **a** and **c** facets, but not for the **s** facet. They discussed qualitatively some of the consequences of higher-neighbor interactions.

In an effort to improve the agreement, we[8] have recently been carrying out Monte Carlo simulations of two- and three-dimensional Ising models that correspond to several facets of hcp lattices, including higher-neighbor interactions. (Simulations on hcp are complicated by the fact that it is not a Bravais lattice.) If the next-nearest-neighbor (NNN) interactions are taken into account, two additional facets of hcp crystals appear: the (1012) and (1210) facets. Since neither of these has yet been observed, it is possible that the NNN interactions may be of little importance in the hcp crystal.[9,10]

The situation is completely different for the bcc crystal. In this structure, we expect the NNN interactions to be considerably more important, since the NNN distance in the bcc lattice is only $2/\sqrt{3}\approx 1.15$ times larger than the nearest neighbor (NN). By comparison, for the sc, fcc, and hcp lattices this ratio is equal to $\sqrt{2}\approx 1.41$. Since the van der Waals force is proportional to r^6, this makes a factor of 3.4 difference. It is therefore significant that the (100) and the (211) facets, whose RT's only occur as the result of higher-neighbor interactions, have been observed[1] for ^{3}He. In view of these observations, we have extended the approximate 2D Ising-model approach to the bcc lattice.

We have studied the (100), (110), (210), and (211) facets of the bcc lattice (Table I). The ratios $R=J_{\mathrm{NNN}}/J_{\mathrm{NN}}$ and $R_1=J_{3\mathrm{NN}}/J_{\mathrm{NN}}$ were considered as parameters. These parameters have the values 0.67 and 0.10, respectively, for the Lennard-Jones potential in a classical bcc crystal (nearest-neighbor distance corresponding to the minimum of the potential well) and approximately 0.42 and 0.05 when the measured ^{3}He interatomic distance, which takes into account zero-point motion, is used. The Hamiltonians for the 2D Ising models corresponding to the four orientations considered are as follows.

TABLE I. Roughening temperatures (units of J_{NN}).

	R	R_1	(110)		(100)		(211)		(210)	
			MC	Analyt.	MC	Analyt.	MC	Analyt.	MC	Analyt.
	0	0		2.269	0	0	0	0		
	0.42	0.05	2.7±0.1		0.8±0.1	0.97	0.63±0.1	0.75	<0.14	0.09
	0.67	0.1	3.3±0.1		1.3±0.1	1.5	0.9±0.1	0.91	<0.22	
$100T_r/T_r(110)$	0.42		100		30	36	24	28	<4.7	
$100T_r/T_r(110)$	0.67		100		39	45	27	28	<6.3	
Experimental results (Ref.10), mK			100		>15;<60		>10;<60		<2.5	

(1) The (100) facet on the lattice shown in Fig. 1, with a staggered magnetic field between A and B sites, has the Hamiltonian

$$\mathcal{H}=-J_{NN}\left[\sum_{ij=NN}\sigma_i\sigma_j+R\sum_{ij=NNN}\sigma_i\sigma_j+4\left(\sum_{i\in A}\sigma_i-\sum_{i\in B}\sigma_i\right)\right]. \quad (1)$$

(2) The (110) facet on the lattice shown in Fig. 2 would be the usual Onsager lattice without NNN bonds. Including NNN it has the Hamiltonian

$$\mathcal{H}=-J_{NN}\left(\sum_{ij=NN}\sigma_i\sigma_j+R\sum_{ij=NNN}\sigma_i\sigma_j\right). \quad (2)$$

(3) The (211) facet on the lattice shown on Fig. 3 (the rectangular Onsager lattice) has the Hamiltonian

$$\mathcal{H}=-J_{NN}\left(\sum_{ij=NN}\sigma_i\sigma_j+R_1\sum_{ij=3NN}\sigma_i\sigma_j\right). \quad (3)$$

(Probably the off-plane sites ought to be taken into account, but it seems that this will only make the model more complicated without changing the result significantly.)

(4) The (210) facet on the lattice shown on Fig. 4, with a staggered magnetic field introduced between A and C sites, has the Hamiltonian

$$\mathcal{H}=-J_{NN}\left[\sum_{ij=NN}\sigma_i\sigma_j+R\sum_{ij=NNN}\sigma_i\sigma_j+(2+R)\left(\sum_{i\in A}\sigma_i-\sum_{i\in B}\sigma_i\right)\right]. \quad (4)$$

In Table I we also compare the results of the numerical simulations with analytical results where these exist. The (110) facet without the NNN interactions is the square Onsager lattice which undergoes a phase transition at $T_c=2.269J_{NN}$. For the (100) facet there is an analytically solvable Ising model which ignores the staggered field correction. This is the square lattice with $J=J_{NNN}$, for which there is a phase transition at $T_c(100)=2.269J_{NNN}$. Thus, $T_c(100)\approx RT_c[(110),\ R=0]$. The model for the (211) facet is a rectangular Onsager lattice which is exactly solvable; the critical temperature is obtained from the equation

$$\sinh(2J_{NN}/T_c)\sinh(2J_{3NN}/T_c)=1, \quad (5)$$

and for $R_1=0.05$ this gives $T_c(211)=0.75J_{NN}=0.33T_c(110,\ R=0)$. The model for the (210) facet can be approximated by the rectangular Onsager lattice with NNN and 6NN for $J_{6NN}/J_{NNN}=0.008$; its transition temperature is $T_c(210)=0.487J_{NNN}=0.205J_{NN}=0.09T_c(110,\ R=0)$.

The simulations were performed using the Metropolis algorithm[9] on a 20×20 lattice sample with periodic boundary conditions. Both smooth and rough initial states were used in order to ensure that equilibration was achieved. About 10^5 steps per site were performed. After equilibration,

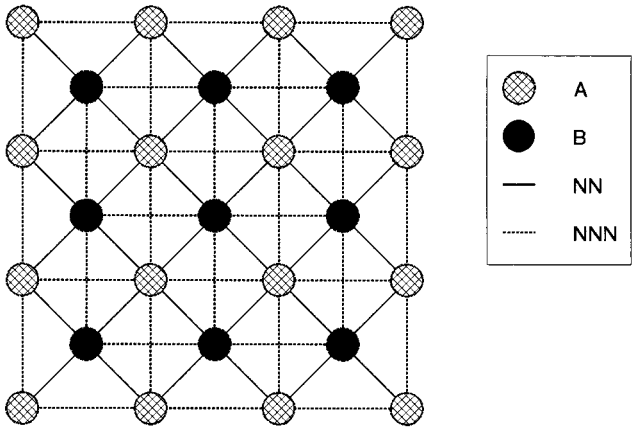

FIG. 1. The 2D Ising model corresponding to the bcc (100) facet. A and B lie in planes at heights differing by half the lattice parameter.

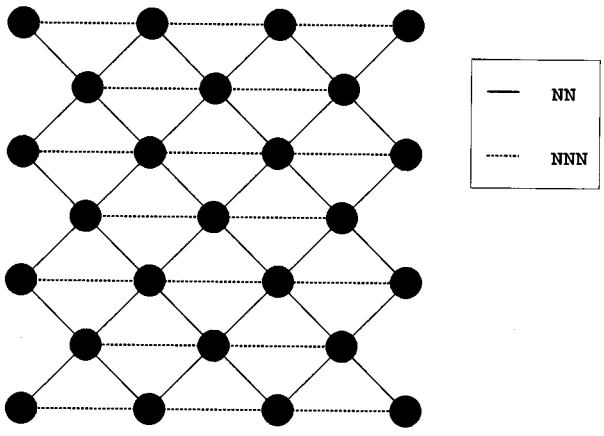

FIG. 2. The 2D Ising model corresponding to the bcc (110) facet.

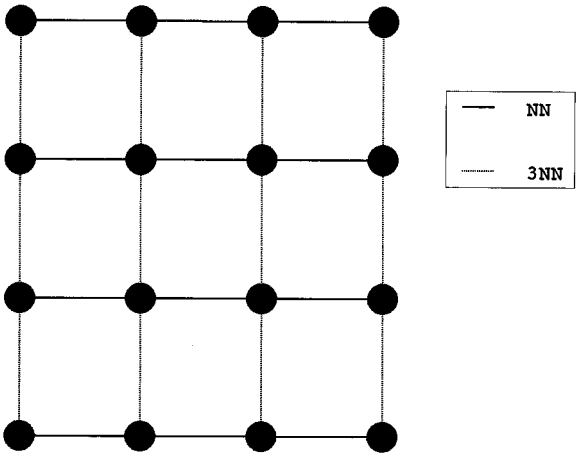

FIG. 3. The 2D Ising model corresponding to the bcc (211) facet.

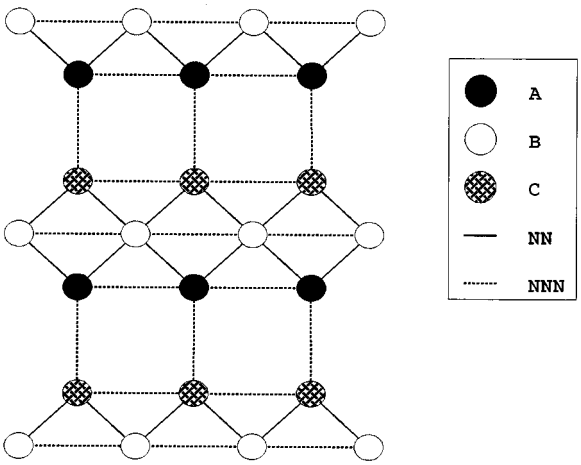

FIG. 4. The 2D Ising model corresponding to the bcc (210) facet. A, B, and C lie in planes at heights separated by 0.22 lattice parameters.

and then after each 200 steps per site, the magnetization was measured and then averaged, with the standard deviation also calculated. At the transition temperature the magnetization fell abruptly to zero, and the standard deviation drastically increased. Above it the standard deviation slowly decreased again. Although this is a relatively primitive approach, comparison with the exactly solved models confirms that good agreement with the transition temperatures calculated via other schemes was achieved.

The values shown in Table I are roughening temperatures obtained by Monte Carlo simulations with $R=0.42$, $R_1=0.05$ and $R=0.67$, $R_1=0.1$. As it was already mentioned, the (211) facet contains no next-nearest neighbor bonds, and third-neighbor bonds have to be taken into account. In addition to these explicit results, we have added analytical values where these are available. The ratios between the transition temperatures have been expressed in percentages so that the values can easily be compared with the experimental limits in mK since (110) facets were observed at about 100 mK. It will be observed that the calculations agree with the experimental limits, but are lower than the estimates from the Kosterlitz-Thouless theory.[4] For the (210) facet where no transition was observed, the simulations gave no evidence of faceting within computation times available at temperatures above those indicated.

We conclude that the results obtained by simulation fit within the experimental limits imposed by the experiments. But their complete verification can come only from more precise experiments with (100), (211), and (210) facets. The agreement of the results with experiment also implies that there must be additional complications for ^{4}He and, in general, the KT theory, experiment, and direct simulation are in good agreement.

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