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Simple model for the equilibrium shape of ^{4}He crystals

M. Touzani
École Normale Supérieure Takaddoum, Boîte Postale 5118, Rabat, Morocco
and Laboratoire de Magnétisme, Université Mohammed V, Faculté des Sciences, av. Ibn Batouta, Boîte Postale 1014, Rabat, Morocco

Michael Wortis
Schlumberger-Doll Research, Ridgefield, Connecticut 06877-4108
and Department of Physics and Materials Research Laboratory, University of Illinois at Urbana-Champaign,
1110 West Green Street, Urbana, Illinois 61801

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A nearest-neighbor Kossel-crystal model accounts for many of the observed features of hcp ^{4}He equilibrium crystal shapes, including the identity of the principal facets, the class of crystal-shape thermal evolution, the macroscopic aspect ratio of the crystal, and the sequence and order of magnitude of faceting temperatures.

I. INTRODUCTION

A number of groups[1-7] have made detailed observations of the shape of macroscopic (~ 1 cm) ^{4}He crystals in coexistence with the superfluid phase at temperatures less than 1.46 K. In this regime the bulk solid is hexagonal close packed (hcp). Above a highest roughening temperature $T_{R_c} = 1.28$ K the crystal shape is everywhere smoothly curved. The two basal-plane $\{0001\}$ facets (the so-called c facets) make their first appearance at T_{R_c} and grow as the temperature is reduced below this value. Between 1.28 K and a second roughening temperature $T_{R_a} \sim 1.0$ K these are the only two facets present; the rest of the crystal surface remains smoothly curved and meets the facets without slope discontinuity.[8] At T_{R_a} the six $\{1\bar{1}00\}$ or a facets appear, perpendicular to the c facets but separated from them and from one another by curved regions. The twelve $\{1\bar{1}01\}$ or s facets show up below a third roughening temperature[5] $T_{R_s} \sim 0.35$ K. Facets continue to grow as the temperature is lowered but remain separated from one another by curved regions. Observations[5] have been extended down to ~ 0.07 K without appearance of further facets. Even at the lowest temperatures reached, significant curved regions remain. It is believed on theoretical grounds[9] that the crystal shape should become completely faceted at temperature $T = 0$ K (only).

The thermal evolution of equilibrium crystal shapes has been studied theoretically for simple model systems,[10-15] and in this context it is believed to be generically understood. There are two types of behavior.[16] "Class A" behavior is like that exhibited by ^{4}He: Faceting is complete only at $T = 0$; for $T > 0$ facets are always separated by curved regions and disappear as temperature is increased, each at its own characteristic roughening temperature.[17] Class A also includes certain metal crystals such as Pb (Refs. 8 and 18) and In[19-21] in coexistence with their vapor; however, mass transport in these systems is much less efficient than it is for ^{4}He, so even for small (~ 1 μm) crystals equilibrium can only be established over a narrow temperature interval near melting. Thus, ^{4}He is at this time the most completely explored example of class A evolution. In "class B" evolution, exhibited, for example, by NaCl,[22] the crystal remains completely faceted up to a nonzero temperature.

The purpose of this paper is to point out that a simple Kossel-crystal model suffices to account remarkably well for many of the observed features of ^{4}He crystal-shape evolution. The model is described in Sec. II, with special emphasis on the way in which its interpretation differs from that of similar models of vapor-crystal coexistence. Sections III and IV deal with $T = 0$ properties and roughening (faceting) temperatures, respectively. Some discussion of possible refinements is included in Sec. V. Inclusion of nearest neighbors only is certainly a gross approximation, and it is not surprising that some features—such as the s-facet roughening temperature—are not well described. Treatment of this model is justified by the principle of doing the simplest things first.

II. MODEL

We take the atoms of the bulk crystalline solid to be situated on the sites of a perfect hcp lattice. We assume that the interfaces between the crystal and the superfluid may be relaxed but are not reconstructed, so the surface atoms can still be indexed to the perfect lattice.[23] Our hypothesis is that the energy of any given microscopic interface configuration is proportional to the number of nearest-neighbor ("dangling") bonds which cross the solid-superfluid boundary. The c/a ratio observed at low temperature[24] for ^{4}He is experimentally indistinguishable from its ideal, spherical-packing value $\sqrt{8/3} = 1.633\ldots$, so it is reasonable to assume that the energy $v/2$ per bond is the same for in-plane and out-of-plane pairs. The factor of $\frac{1}{2}$ introduced here makes v the energy required per broken nearest-neighbor crystalline bond to cleave a macroscopic crystal (in coexistence with its superfluid) into two parts along a specified interface, since in this process each crystalline bond broken leaves two dangling bonds, one on each of the two resulting interfaces. In Sec. IV we shall briefly consider the effect of relaxing the assumptions of in-plane and out-of-plane equivalence and nearest-neighbor-only interactions.

Operationally this model is just the hcp version of the "broken-bond" or Kossel-crystal models which have been extensively used (especially at $T=0$) to study solid-gas interfaces.[25,26] The present context is somewhat different, however, in that (i) the coexisting fluid here is a condensed phase, reduced in density from the solid by only about[27] 10%, and (ii) solid formation in ^{4}He is at these temperatures driven by the external pressure (P). This means that the parameter v cannot be thought of as equal (even approximately) to the energy required to separate a pair of atoms from their crystalline nearest-neighbor distance off to infinity. Indeed, for ^{4}He the (negative) potential energy of formation of the solid is more than off-set by the (positive) kinetic energy, so that at $P=T=0$ the solid is unstable. When the solid does form, at $P_0 \approx 25$ atm, the energy change across the transition is related to the volume change by $\Delta E \approx -P_0 \Delta V$ (since the entropy term is small at low temperature), so the bulk energy of the superfluid phase is actually lower than that of the solid phase, quite the reverse of the situation at ordinary gas-solid coexistence. Thus, although the interface energy per unit area is required to be positive (for stable phase separation), there is no simple rule relating v to bulk parameters [analogous, for example, to[28] $v \sim L$ (latent heat)]. We shall argue only that

$$v \sim V(a_{\text{liquid}}) - V(a) \ , \tag{1}$$

where $V(r)$ is the He-He pair potential, a is the nearest-neighbor spacing in the solid[24] ($a = 3.57$ Å at $T=0$), and a_{liquid} is a characteristic interatomic spacing in the superfluid. Equation (1) expresses the expectation that the relevant "bond-breaking" energy should be comparable to the energy required to increase the pair spacing from a to the larger value a_{liquid}. Kinetic-energy effects, local relaxation in the solid, structure in the near-surface fluid profile, etc., may all be expected to modify this estimate by factors of order unity. In Sec. IV, we shall need a value for v to calculate T_{R_c}. To obtain a numerical estimate, we may put

$$a_{\text{liquid}}/a \sim (V_{\text{liquid}}/V_{\text{solid}})^{1/3}$$

(the ratio of molar volumes[27]) and use for $V(r)$ the Aziz potential.[29] This gives $v \simeq 1.15$ K. Alternatively, as we shall see in Sec. IV, it is possible to fit v to the observed value of T_{R_c}. This procedure leads to a similar estimate for v.

III. EQUILIBRIUM CRYSTAL SHAPE AT $T=0$

To find an equilibrium crystal shape (ECS) at temperature T, it is necessary to calculate the interfacial free energy per unit area $f_i(T,\hat{\mathbf{m}})$ as a function of interface orientation $\hat{\mathbf{m}}$ (relative to the bulk-crystal axes) and then to perform the Wulff construction.[30,31] At $T=0$ the calculation reduces to counting the number of broken bonds per unit interfacial area.[32] This calculation has been carried out for the hcp lattice by a number of authors.[25,33,34] Since the explicit forms do not seem to be available in the literature, we take the liberty of quoting them here. For the c, a, and s facets, we find,

$$f_i(T=0,c) = \sqrt{3}\frac{v}{a^2} \ , \tag{2}$$

$$f_i(T=0,a) = \frac{3\sqrt{6}}{4}\frac{v}{a^2} \ , \tag{3}$$

$$f_i(T=0,s) = \frac{7\sqrt{123}}{41}\frac{v}{a^2} \ . \tag{4}$$

Quite generally, the three-dimensional plot $f_i(T=0,\hat{m})$ is composed of several distinct intersecting surfaces,[31] which we shall index j, each with the equation

$$f_i(T=0,\hat{m}) = 2\mathbf{C}_j \cdot \hat{m} \ , \tag{5}$$

corresponding to a sphere of radius C_j centered at $\mathbf{C}_j$. For the ideal hcp lattice there are 24 such spherical regions; however, because of the symmetry, only two are independent. These two cover the fundamental stereographic triangle as shown in Fig. 1 and have centers at,

$$\mathbf{C}_1 = \frac{1}{2}(\sqrt{2},0,\sqrt{3})\frac{v}{a^2} \tag{6}$$

and

$$\mathbf{C}_2 = \frac{1}{2}\left[\frac{3}{\sqrt{2}},0,\frac{1}{\sqrt{3}}\right]\frac{v}{a^2} \ . \tag{7}$$

The ECS which follows from Eqs. (2)–(7) is shown in Fig. 2.[35] The form is an hexagonal prism exhibiting c and a facets, truncated perpendicular to $[16\,\overline{16}\,9]$ and equivalent directions to form the s facets. No other facets appear on the ECS. Note that these are precisely the facets observed in experiments. The aspect ratio (height/width) is 0.94 or 0.82, as the crystal is viewed

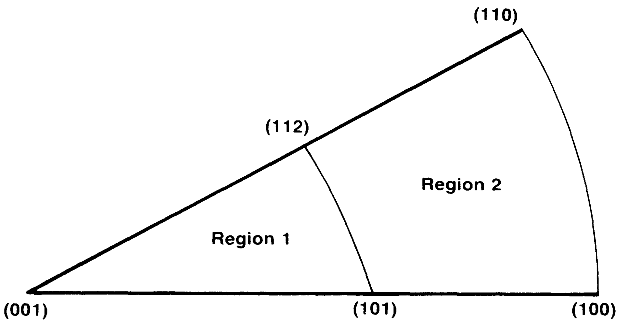

FIG. 1. The fundamental stereographic triangle, showing the regions covered by the spherical surfaces 1 and 2 given by Eqs. (5)–(7).

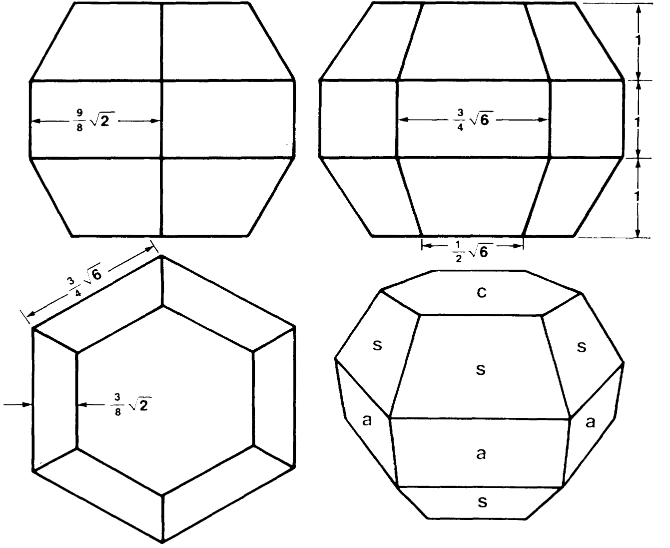

FIG. 2. Calculated equilibrium shape of the nearest-neighbor hcp crystal at $T=0$. Lower right shows a perspective sketch.

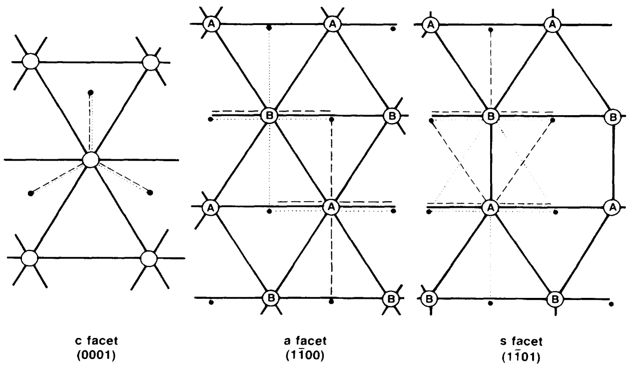

FIG. 3. Ising approximations to RSOS models for the c, a, and s interfaces, as viewed along the directions [001], $[1\bar{1}0]$, and $[1\bar{1}0]$, respectively. Open circles show positions in the layer ($z=1$) which may be either occupied or unoccupied. Solid lines connect in-layer nearest neighbors. Black dots give positions of atoms in the layer below (or above). For the a and s facets, there are two inequivalent classes of sites, A and B, in each layer. The full (12-fold) coordination of representative sites is shown. Dashed lines connect to neighboring sites in the layer above; dotted lines, to those in the layer below. Unequal numbers of "up" and "down" neighbors leads to a magnetic field in the equivalent Ising models.

along the $[1\bar{1}0]$ or [100] directions, respectively. There are no measurements of the equilibrium aspect ratio at low[36] T; however, observations[37] at 1.26 K which are probably near equilibrium show an aspect ratio of about 0.76, which is in the right range. Finally, all the $T=0$ ECS edges are "marginal" in the sense that Wulff planes of all orientations touch the ECS, so each edge is highly degenerate. It is a consequence of this degeneracy that the edges are rounded at any $T>0$, corresponding to class A evolution,[11,14] as is (apparently) seen in experiment.

IV. FACET ROUGHENING

As the temperature is raised above zero, each facet disappears at a "faceting" temperature, characterized by the disappearance of the corresponding cusp in the Wulff plot. Because the slope of the cusp is the step free energy per unit length,[10,38] this faceting temperature is just the roughening temperature of the face in question.

Roughening temperatures of the three $T=0$ facets can be estimated via appropriate restricted solid-on-solid (RSOS) models. For example, for the c facet, each basal plane consists of a triangular lattice, with adjacent planes in the $ABAB$ sequence, as shown in Fig. 3. The "restriction" is simply that a site in layer $z+1$ can only be occupied if all its near neighbors in layer z are already present. The analogous model for the bcc lattice [the body-centered-solid-on-solid (BCSOS) model] was solved exactly by van Beijeren[39] and gives a description of the critical behavior near the faceting transition which is generically correct (XY-like). Furthermore, the RSOS estimate of T_R is probably excellent, since the neglect of overhangs and vacancies is not expected to be numerically important. With these considerations in mind, we adopt the RSOS estimate of T_R. Unfortunately, the triangular (hcp) RSOS model has not to the best of our knowledge been solved, even numerically, so it is necessary to resort to further approximation. We recall that the two-layer SOS model (completely filled $z=0$ plane, partially filled $z=1$ plane) is equivalent to a triangular Ising ferromagnet with Hamiltonian,[40]

$$H_c=-\frac{v}{4}\sum_{\langle i,j\rangle}\sigma_i\sigma_j+\text{const},\quad \sigma_i=\pm 1\ , \tag{8}$$

where the sum $\langle i,j\rangle$ is over nearest-neighbor pairs. Although the critical behavior of this Ising model is quite different from that of the corresponding RSOS model, the Ising T_c is probably a good approximation[41] to both the true T_R and T_R (RSOS). This T_c is known exactly,[42]

$$kT_c(\text{Ising})=3.641\frac{v}{4}\simeq kT_{R_c}\ . \tag{9}$$

Using $v\sim 1.15$ K from Sec. II leads us to estimate $T_{R_c}\simeq 1.05$ K, in good correspondence with the observed value. Although this level of agreement may be fortuitous,[29] it does lend some credence to the model. Alternatively, we may use Eq. (9) in reverse, inserting the observed T_{R_c} and finding $v\simeq 1.41$ K.

Other facets lead in a similar way to (different) Ising estimates for T_R. For the a facet, the Ising lattice is still triangular but, because alternate rows of atoms have different numbers of "up" and "down" nearest neighbors, a staggered magnetic field $h_s=v/2$ now appears, switching sign from each row to the next (see Fig. 3),

$$H_a=-\frac{v}{4}\sum_{\langle i,j\rangle}\sigma_i\sigma_j+\frac{v}{2}\left[\sum_{i\in A}\sigma_i-\sum_{i\in B}\sigma_i\right]+\text{const}\ . \tag{10}$$

The critical temperature of this model is not known exactly; however, it is certainly less than the value (9) (since the staggered field competes with the ferromagnetic order) and may be estimated by taking the ratio $T_c(h_s=v/2)/T_c(h_s=0)$ of the mean-field critical temperatures with and without the field term. This calculation leads to the prediction (independent of v) $T_{R_a}/T_{R_c}\simeq 0.93$, in crude agreement with the observed value of 0.78.

Finally, the s facet leads to a staggered-field Ising model on the $q=5$-coordinated "brickwork" lattice, shown in Fig. 3,

$$H_s=-\frac{v}{4}\sum_{\langle i,j\rangle}\sigma_i\sigma_j+\frac{v}{4}\left[\sum_{i\in A}\sigma_i-\sum_{i\in B}\sigma_i\right]+\text{const}\ . \qquad (11)$$

This model has been solved exactly at zero field and gives[43] $kT_c(h_s=0)=(2/\ln 2)(v/4)$. Scaling with the mean-field ratio for this lattice, $T_c(h_s=v/4)/T_c(h_s=0)=0.971$, leads us to the prediction (independent of v) $T_{R_s}/T_{R_c}\simeq 0.77$. This gives correctly the ordering $T_{R_s}<T_{R_a}<T_{R_c}$ but is almost a factor of three higher than the experimental value $0.35/1.28=0.27$. It is possible that this discrepancy may be at least partially accounted for by (i) inaccuracy in the experimental T_{R_s} (it is hard to pinpoint the first appearance of the s facet) or (ii) inadequacy in the Ising estimates of the RSOS T_c. Probably, however, it indicates the need for refinement of the simple, one-parameter model.

V. DISCUSSION

The simplest nearest-neighbor model seems to account well for many of the main experimental observations, including (i) the identity of the principal facets, (ii) the class of thermal evolution of the ECS, (iii) the macroscopic aspect ratio of the crystal, (iv) the sequence of faceting temperatures, and (v) the order of magnitude of the roughening temperatures T_{R_c} and T_{R_a}. Of course, it would be preferable not to have to rely on the Ising estimates of the RSOS T_R's and the various additional approximations invoked in treating the Ising models. Improvements along these lines are in progress.[44]

The poor value obtained for T_{R_s} suggests that refinement of the model may be necessary. Two avenues immediately suggest themselves: (i) inclusion of asymmetry between basal-plane and out-of-plane nearest-neighbor bond strengths and (ii) inclusion of further-neighbor interaction. The ideal value observed for the c/a ratio suggests that (i) is not important, so we concentrate on (ii). Each atom has six next-nearest neighbors (NNN's) situated at distance $a\sqrt{2}$. The He-He potential is attractive at NNN separation, and we may estimate[45] [in analogy to Eq. (1)]

$$v_{\text{NNN}}\sim V(\sqrt{2}a_{\text{liquid}})-V(\sqrt{2}a)\simeq 0.122\ \text{K}\ . \qquad (12)$$

The effect of NNN attraction on the $T=0$ crystal shape has been studied by Stranski and Kaischew,[25,33,46] who find that the $\{1\bar{1}02\}$ and $\{11\bar{2}0\}$ facets appear. Class A thermal evolution is still expected as long as $v_{\text{NNN}}>0$. Since these new facets have not yet been seen, it is important to estimate their roughening temperatures. Because these facets are absent for $v_{\text{NNN}}=0$, it is natural to expect,

$$T_R(1\bar{1}02)/T_{R_c}\sim T_R(11\bar{2}0)/T_{R_c}\sim v_{\text{NNN}}/v\sim 1/9\ , \qquad (13)$$

which would lead to roughening temperatures in the vicinity of 0.1 K. This is, of course, only an order-of-magnitude estimate; however, it suggests that new facets should appear near the lower limit of present observations.[5] It is tempting to think that the critical slowing down reported by Puech *et al.*[47] at 0.21 K might correspond to the appearance of one of these facets. Whether the next-nearest-neighbor interactions could play a role in reducing the step free energy for the s facet is not yet clear.

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