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Equilibrium shape of ^{4}He crystal surfaces near critical orientations

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Abstract. **Conditions for applying mean field theory to the thermodynamics of the ^{4}He crystal surface are determined. Although the faceting transition itself is of the Berezinskii–Kosterlitz–Thouless type, the thermodynamic potential outside a narrow neighborhood of the transition temperature can be expanded in the spirit of the Landau theory of second-order phase transitions. A Ginzburg–Levanyuk parameter is found. The singular behavior of the surface stiffness near critical directions observed for essentially noncritical temperatures is explained.**

Keywords: quantum crystals, phase transitions, surface phenomena, Berezinskii–Kosterlitz–Thouless transitions

Yurii Vasil'evich Kopaev is recognized for his outstanding contribution to the theory of phase transitions. In particular, Keldysh and Kopaev's [1] model of an excitonic dielectric is effectively used to describe metal–dielectric phase transitions in solids. Kopaev showed that the excitonic dielectric model describes a wide variety of new states, among them orbital antiferromagnetism and toroidal ordering. It seems natural that the memory of Kopaev be honored by publishing a study on the physics of peculiar phase transitions related to a change in the equilibrium shape of a crystal. Specifically, in this paper we discuss phase transitions that cause a crystal to facet as the temperature is decreased. These 'roughening' transitions are described by the theory of Berezinskii, Kosterlitz, and Thouless (BKT) [2]. In [3], one of the present authors proposed a 'mean field' theory of faceting transitions, which is similar to the Landau theory of second-order transitions. It has been argued (see [4, 5]) that the mean field theory has zero applicability because of the significant role of fluctuations.

In this paper (see also Ref. [6]), based on the analysis of experimental data on the properties of ^{4}He crystal surfaces, we show that on the contrary, the applicability of mean field theory is very wide. The theory is inapplicable only in a very narrow domain around the critical temperature. The relation between the BKT theory and the mean field theory is similar to that between the BKT theory and the Ginzburg–Landau theory for superconducting films (see, e.g., Ref. [7]).

In the simplest case of one-dimensional geometry, the mean field theory is developed by introducing the surface thermodynamic potential f related to the surface energy per unit surface area α as $f = \alpha\sqrt{1+h^2}$, where $h = \partial z/\partial x = \tan\theta$ is an angular variable, θ is the angle between the surface and the basal plane of the crystal, and $z = z(x)$ is the crystal surface equation. In equilibrium, the relation to the surface energy is

$$\lambda z(x) = \tilde{f}(-\lambda x)\,, \tag{1}$$

where $\tilde{f} = \tilde{f}(\eta) = f - \eta h$ is the Legendre transform of the potential $f(h)$, $\eta = \partial f/\partial h$, and λ is a constant.

The mean field theory is based on expanding the potential $\tilde{f}$ for vicinal ($h \ll 1$) surfaces in powers of η,

$$\tilde{f} = -\frac{a}{2}\,\eta^2 - \frac{b}{4}\,\eta^4\,, \tag{2}$$

where $a = a(T)$ is a function of the temperature and b is a constant. To determine the conditions of applicability of expansion (2), we pass to the dimensionless variables

$$\tilde{f}' = b^{1/3}\tilde{f}\,, \quad \eta' = b^{1/3}\eta\,.$$

We have

$$\tilde{f}' = -\frac{1}{2}\left(ab^{-1/3}\right)\eta'^2 - \frac{1}{4}\,\eta'^4\,. \tag{3}$$

The angular parameter is expressed as

$$h = -\frac{\partial\tilde{f}}{\partial\eta} = a\eta + b\eta^3 = \left(ab^{-1/3}\right)\eta' + \eta'^3\,. \tag{4}$$

If the condition

$$\left|ab^{-1/3}\right| \ll 1 \tag{5}$$

is satisfied, expansion (3) is valid for $\eta' \ll 1$ or, equivalently, $h \ll 1$.

A direct way of finding the coefficients in expansion (3) is to monitor the shape of the equilibrium surface $h(x)$. From relation (1), it follows that

$$h(x) = -a\lambda x - b(\lambda x)^3\,. \tag{6}$$

Babkin, Kopeliovich, and Parshin [8, Fig. 3a] performed such measurements for vicinal directions very near (both above

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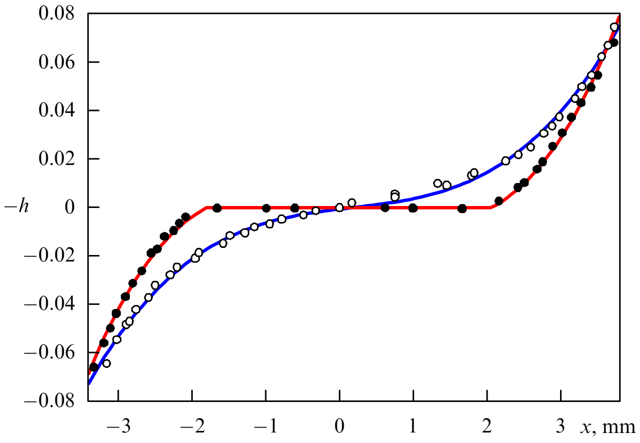

Figure 1. Equilibrium crystal shape $h(x)$ for $T > T_R$ (circles) and $T < T_R$ (black dots) (see Fig. 3a in Ref. [8]). The curves are put into correspondence with expansion (6), with the best fit obtained for $a\lambda|_{T>T_R} = 3.6 \times 10^{-3}$ mm^{-1}, $b\lambda^3|_{T>T_R} = 1.3 \times 10^{-3}$ mm^{-3}, $a\lambda|_{T<T_R} = -8.3 \times 10^{-3}$ mm^{-1}, and $b\lambda^3|_{T<T_R} = 2.2 \times 10^{-3}$ mm^{-3}.

and below) the faceting phase transition point T_R. It turns out that outside a narrow region $\delta T \lesssim 0.01$ near the critical temperature, the shape of the crystal is independent of the temperature (we note that crystal shapes are evidently different for $T > T_R$ and $T < T_R$). This implies that the coefficient a is temperature-dependent only in this region, where it is a positive constant $a = a_h$ for $T > T_R$ and a negative constant $a = -a_l$ for $T < T_R$. Results for two particular samples, with

$$a_h b^{-1/3} = 0.03 \tag{7}$$

and

$$a_l b^{-1/3} = 0.06\,, \tag{8}$$

are given in Fig. 1.

We now show that expansion (2) can be used to describe the still unexplained features of the angular dependence of the surface rigidity γ (Fig. 2), which were experimentally observed by Andreeva and Keshishev [9] close to the special facets (0001) and $(10\bar{1}0)$ below T_R.

We consider the ^{4}He crystal's basal face (0001) perpendicular to the sixth-order symmetry axis. The faceting temperature $T_R \approx 1.28$ K itself is determined by the universal relation from the BKT phase transition theory,

$$T_R = \frac{2}{\pi}\,\gamma d^2\,, \tag{9}$$

where $d \approx 3$ Å is the lattice constant normal to the face and

$$\gamma = \alpha + \frac{\partial^2 \alpha}{\partial \theta^2} = \frac{\partial^2 f}{\partial h^2} = \frac{\partial \eta}{\partial h} \tag{10}$$

is the surface rigidity at $T = T_R$ and $h = \theta = 0$. The mean field theory critical temperature T_c is determined by the vanishing condition for the second-order coefficient in expansion (2), $a(T_c) = 0$, and hence sufficiently close to the critical temperature, $|T - T_c| \ll \delta T$, we have $a = a_0 t$, where $t = (T - T_c)/T_c$.

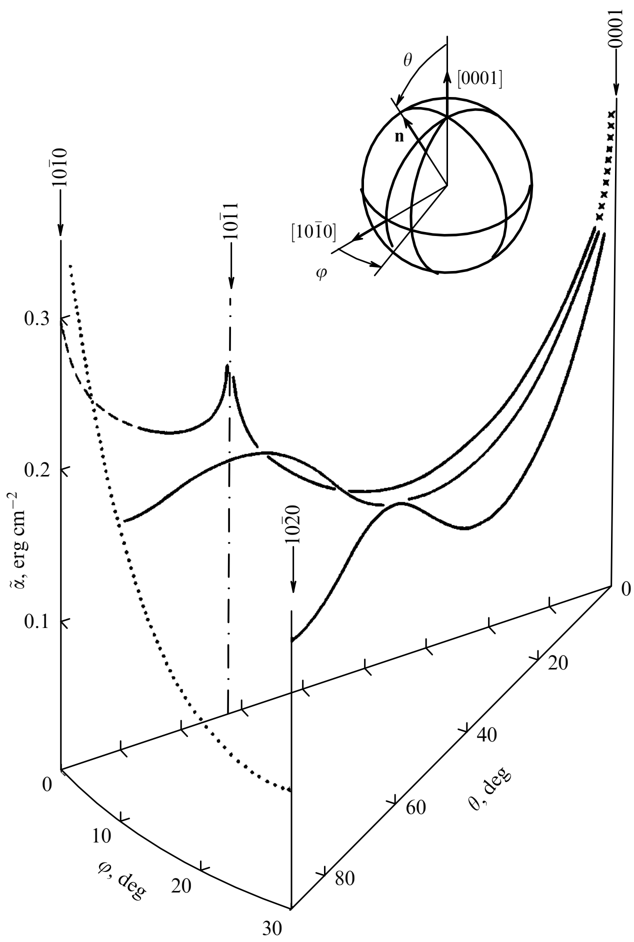

Figure 2. Angular dependence of surface rigidity (from Ref. [9]).

Assuming T_R to be close to T_c, we use Eqn (2) to find $\gamma = (a_0 t)^{-1}$ and

$$t_R = \frac{T_R - T_c}{T_c} = \frac{2}{\pi}\,\frac{d^2}{a_0 T_c}\,.$$

Thus, the condition for the theory under discussion to apply is $t > t_R$, and the parameter

$$\mathrm{Gi} \equiv t_R = \frac{2d^2}{\pi a_0 T_c} \ll 1 \tag{11}$$

plays the role of the Ginzburg–Landau parameter in the theory of second-order phase transitions [7].

Detailed experimental data on the angular dependence of the surface rigidity (10) at low ($T < T_R$) temperatures are presented in theses [10] (see Fig. 19 therein). Expansion (4) allows calculating this dependence, with the result

$$\gamma = \left(\frac{\partial h}{\partial \eta}\right)^{-1} = \left(3b\eta^2 - a_l\right)^{-1}. \tag{12}$$

From Eqns (4) and (12), the relation between γ and the angular parameter h follows as

$$\bar{h} = \left(\frac{\bar{\gamma}+1}{3\bar{\gamma}}\right)^{3/2} - \left(\frac{\bar{\gamma}+1}{3\bar{\gamma}}\right)^{1/2}, \tag{13}$$

where $\bar{h} = (a_l^3/b)^{-1/2} h$, $\bar{\gamma} = a_l \gamma$. For $\bar{h} \ll 1$, we have $\bar{\gamma} \approx 1/2 - 3/4\,\bar{h}$; for $\bar{h} \gg 1$, the rigidity decreases in proportion to $h^{-2/3}$: $\bar{\gamma} \approx 1/3\,\bar{h}^{-2/3}$.

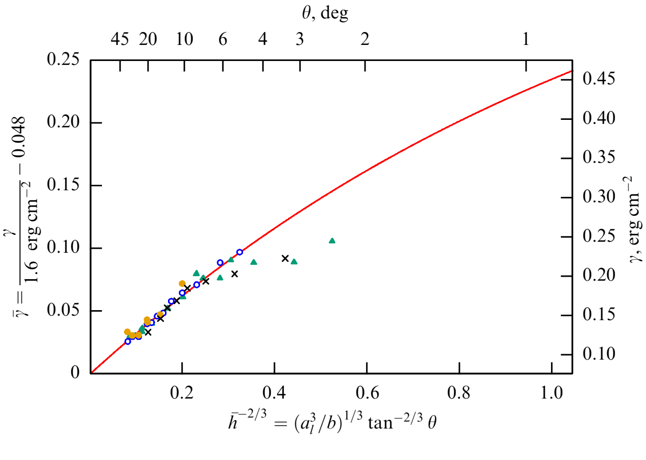

Figure 3. Angular dependence of surface rigidity for four samples from the experimental data of Andreeva and Keshishev (see Fig. 9 in Ref. [10]) and theoretical curve (11).

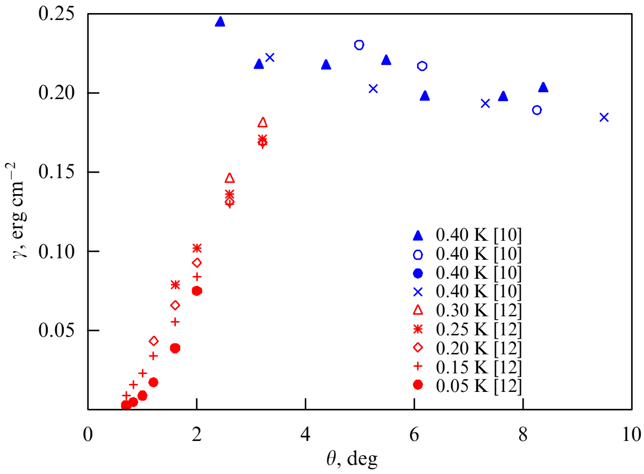

Figure 4. Angular dependence of surface rigidity for vicinal directions at low temperatures (from the data in Refs [10, 12]).

For $T < T_{\mathrm{R}}$, the value $(a_l^3/b)^{-1/2} = 62.5$ follows from Eqn (8). The parameter

$$a_l^{-1} = 1.6\ \mathrm{erg\ cm^{-2}} \tag{14}$$

is determined from the best fit to the experimental data. The corresponding dependence (13) is plotted in Fig. 3. We note that the minimum angle for which the experimental points fit curve (13) well is precisely the one corresponding to constraint (16) on the applicability region of mean field theory (see also Fig. 5 below).

The fact mentioned above that the surface rigidity is temperature independent outside the immediate neighborhood of the critical temperature implies that the parameter a is temperature dependent only in this region, where it changes by an amount of the order of a_l, i.e., $a_0 \gtrsim a_l(T_{\mathrm{c}}/\delta T)$. Using Eqn (14), we estimate the value of Gi from Eqn (11) as

$$\mathrm{Gi} \lesssim \frac{2d^2\delta T}{\pi a_l T_{\mathrm{c}}^2} \sim 0.1\,.$$

The vicinal surface of a crystal in the zero-temperature limit consists of a series of sparse steps of height d on a symmetric face [11], with the consequence that the surface rigidity tends to zero as $\theta \to 0$ (Fig. 4). This picture breaks down if fluctuations on the surface 'wash out' the discreteness of the crystal structure and the concept of a finite-height step itself becomes meaningless. In accordance with the universal relation (9), this should arguably occur at

$$T \gtrsim T_{\mathrm{R}}(\theta) \equiv \frac{2d^2\gamma(\theta)}{\pi}\,, \tag{15}$$

where d is independent of θ, and the surface rigidity $\gamma(\theta)$ can be determined from Eqn (13). Thus, at temperatures below the faceting point, the applicability region of the theory under discussion is determined by the condition

$$\begin{aligned}\bar{h} &\gtrsim \left(\frac{\bar{\gamma}+1}{3\bar{\gamma}}\right)^{3/2} - \left(\frac{\bar{\gamma}+1}{3\bar{\gamma}}\right)^{1/2} \\ &= \left(\frac{1}{3} + \frac{2d^2}{3\pi a_l T}\right)^{3/2} - \left(\frac{1}{3} + \frac{2d^2}{3\pi a_l T}\right)^{1/2}.\end{aligned} \tag{16}$$

Figure 5 shows the corresponding set on the (T, θ) plane.

Our analysis of the observed surface shape does not include the effect of gravity. The equilibrium condition in the field of gravity g has the form (the subscript g indicates the inclusion of gravity)

$$\frac{\partial \eta_g}{\partial x} = -\lambda + g z_g\,\Delta\rho\,, \tag{17}$$

where $\Delta\rho$ is the density difference between the crystal and the liquid. Integrating in the leading approximation over x yields

$$\eta_g = \int(-\lambda + g\Delta\rho z_g)\,\mathrm{d}x \approx -\lambda\left(x + \frac{ag\Delta\rho}{6}\,x^3\right). \tag{18}$$

The surface profile z_g itself can be obtained in the same approximation by integrating the relation

$$\begin{aligned}\frac{\partial z_g}{\partial \eta_g} &= \frac{\partial z_g}{\partial x}\,\frac{\partial x}{\partial \eta_g} = \frac{h}{-\lambda + g z_g \Delta\rho} \\ &\approx \frac{h}{-\lambda}\left(1 + \frac{g z \Delta\rho}{\lambda}\right) = \frac{\partial}{\partial \eta}\left(\frac{\tilde{f}}{\lambda} + \frac{g\tilde{f}^2\Delta\rho}{2\lambda^3}\right)\end{aligned} \tag{19}$$

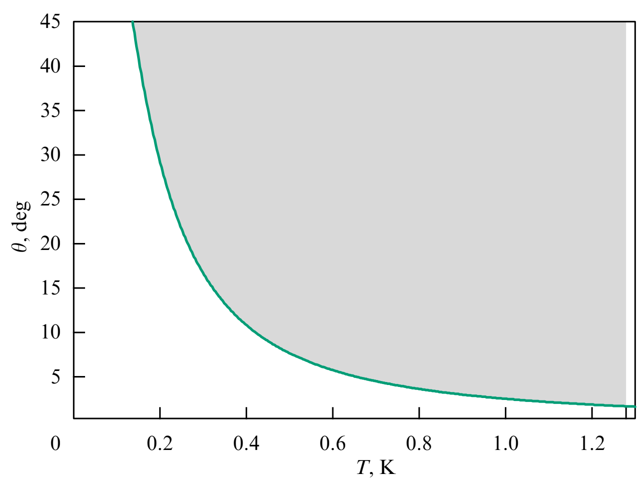

Figure 5. Constraint on the region of applicability of the mean field theory in accordance with Eqn (16).

to yield

$$z_g \approx \frac{1}{\lambda}\,\tilde{f}(\eta_g) + \frac{g\Delta\rho}{2\lambda^3}\,\tilde{f}^{\,2}(\eta) \approx z - \lambda\,\frac{a^2 g\Delta\rho}{24}\,x^4$$
$$= -\frac{a\lambda}{2}\,x^2 - \frac{b\lambda^3}{4}\,x^4 - \lambda\,\frac{a^2 g\Delta\rho}{24}\,x^4\,. \qquad (20)$$

Thus, the condition that allows disregarding the force of gravity is

$$\epsilon \equiv \frac{a^2 g\Delta\rho}{6b\lambda^2} \ll 1\,. \qquad (21)$$

Under the conditions considered here, the parameter ϵ can be estimated by using Eqn (14) and the data from the legend to Fig. 1 to give $\epsilon \approx 0.07$.

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