How should we understand curved facets?

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Babkin et al have found a small curvature in facets of ^{4}He crystals. As a possible explanation they consider a model where the curvature arises from thermally activated defects previously studied by Andreev. We criticize this model, and suggest that the curving arises from pinning of steps near the facet edge.

1. INTRODUCTION

The interface between solid and liquid ^{4}He has recently been studied by Babkin *et al.*[1] By measuring optically the neighborhood of the facet edge, they made the surprising discovery that the facet appeared to be curved. The authors also considered various models in order to understand the observations. In particular, they discussed that the curving may arise from thermally activated dislocation half-loops terminating to the surface. Previously Andreev had argued that such defects destroy the equilibrium faceting of crystals.[2,3]

The purpose of this letter is to show that the theory presented in Refs. 1-3 suffers from an improper definition of a facet. A more useful definition is based on the long-range order of the underlying crystal. Because the long-range order is unaffected by point defects such as dislocation loops, these defects cannot give rise to any bending of the facet. In order to explain the observed curving, I suggest that it arises from pinning of steps near the facet edge.

2. FACETS AND LONG-RANGE ORDER

We study a surface of a crystal parallel to a crystallographic plane. In equilibrium at zero temperature, such a surface is expected to be atomically

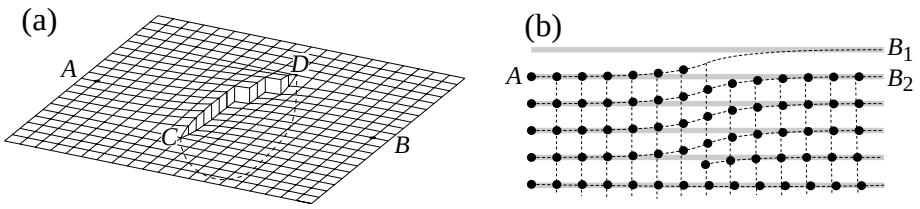

Fig. 1. A step in the crystal surface associated with a dislocation half ring: (a) a view on the surface and (b) cross section along the line AB.

smooth and flat. At any nonzero temperature T, there appear defects proportional to the Boltzmann factor $\exp(-E/kT)$, where E is the energy of the defect. Let us consider a defect depicted in Fig. 1. It has a step of finite length on the surface. The endpoints of the step are connected by a dislocation inside of the crystal. It was argued in Ref. 2 that such defects cause that all equilibrium surfaces are non-faceted at any $T > 0$. The argument goes as follows. Between two points A and B one chooses a straight path on the surface of the crystal. Along this path one tries to identify the unit cells which may be elastically distorted. One then defines a "growth displacement" ζ by counting the number of upward steps minus the number of downward steps. One finds that $\Delta\zeta = \zeta(A) - \zeta(B) = -1$ in the case of Fig. 1. There will be many such defects on the line AB when the points A and B are far from each other. Thus one finds a divergent correlation $< [\zeta(\mathbf{r}) - \zeta(\mathbf{0})]^2 > \propto r$. This was interpreted as evidence that the crystal surface is atomically rough.[2] Using similar arguments it was deduced in Ref. 3 that also defects inside of the crystal destroy the facets in equilibrium.

The reason for the failure of the argument above is that ζ is not a proper quantity to discriminate between a facet and a rough surface. Instead, the definition of a facet should be based on the long-range order of the underlying crystal. The long-range order defines crystallographic planes, which are denoted by shading in Fig. 1b. If most of the atoms at the surface are nearest to a single crystallographic plane, it is natural to define it as a facet. In this view the dislocation half-loop is only a localized defect on the facet because the surface atoms at A and B belong to the same crystallographic plane in spite of $\Delta\zeta = -1$. The theory of the roughening transition considers the surface only on a long range and all localized defects are already included in it.[4]

The long-range order of a crystal is essential to the argument above. It has been studied some time ago that localized defects do not disturb the long-range order of a three dimensional crystal.[5] More precisely, there is a long-range order in the crystal for any fixed but statistically relevant

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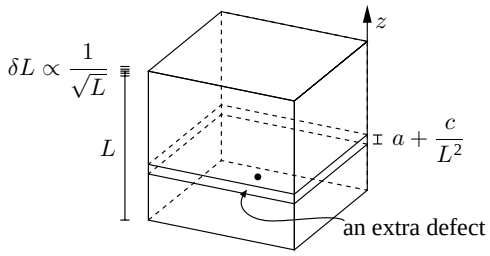

Fig. 2. Illustration that point defects do not destroy long-range order.

distribution of defects. Although this seems to be common knowledge, we demonstrate it here by a simple model because it clarifies the argument presented above.

Let us consider a cubic piece of a crystal, see Fig. 2. In the z direction it consists of L/a two-dimensional atomic layers, where a is the lattice constant. The positions of the layers can be defined according to the center of mass of the atoms belonging to each layer. In thermal equilibrium there is a density n of defects present. It is convenient to consider an interstitial atom between two crystal planes, but any localized defect will lead to the same conclusion. A uniform distribution of such defects leads to an expansion of the crystal lattice relative to a lattice without defects. In order to determine the fluctuations we consider one extra defect relative to the uniformly distributed defects. This obviously increases the distance between the neighboring layers by a quantity that is inversely proportional to the area of the layers, $\Delta u \propto L^{-2}$. The fluctuation in the number of defects is proportional to the square root of the average number: $\delta N \propto \sqrt{N} = \sqrt{nL^3}$. Thus the total fluctuation in the distance between the top and bottom layers $\delta L = \delta N \Delta u \propto 1/\sqrt{L}$. Thus the larger the crystal, the more precisely are the distances between the crystal planes defined.

A very similar model can demonstrate that thermal fluctuations do not destroy the long-range order of a crystal. It is also instructive to generalize these models to 1 and 2 dimensional solids.

3. PINNING OF STEPS

Very accurate studies on the liquid-solid interface of ^{4}He was recently made by Babkin *et al.*[1] The crystal shape was studied interferometrically in the center part of the round container shown in Fig. 3. The c facet of the hexagonal crystal was tilted by a small angle τ with respect to the horizontal direction. In the slope of the surface they found a clear change, which we call here the facet edge. The curved surface on the right hand side can

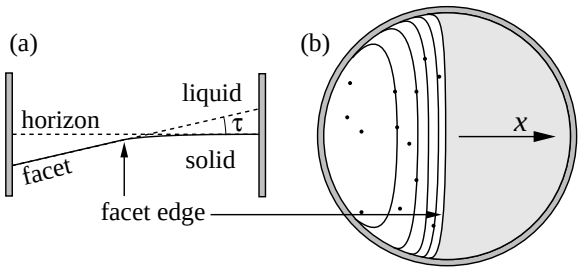

Fig. 3. Schematic representation of the experiment by Babkin *et al*:[1] (a) cross sectional side view, and (b) top view. The steps in the facet are shown by solid lines in (b) and dots denote possible pinning centers.

rather accurately be understood by a surface stiffness that vanishes linearly with the angle $\phi = d\zeta/dx$ measured relative to the facet plane.[6] However, they found that the surface was slightly convex also on the facet side. The deviation ζ from a straight facet (not visible on the scale of Fig. 3) was fitted by an exponential $\zeta(x) = \zeta_0 \exp(x/x_0)$.

As a possible explanation for the curving of the facet, Babkin *et al* suggested a model based on Ref. 2. As I argued in Section 2, this does not provide a viable explanation. Below I describe an explanation based on pinning of steps.

Let us consider an elementary step in the facet.[7] The force on a free step is given by $f = (\rho_\mathrm{s} - \rho_\mathrm{l}) g a \ell h$, where ρ_s and ρ_l are the solid and liquid densities, g the gravity constant, a the step height, ℓ the length of the step, and h the depth measured from the horizon (Fig. 3). This gravity force is very weak near the facet edge. The pinning energy ΔU that is needed to stop one whole step is on the order of 0.3 K (w/a), where w is the range of the pinning potential. Thus a few vacancies in the surface might be sufficient to stop one step.

Suppose the steps jump from one pinned configuration to another by thermal fluctuations, similar to flux creep in superconductors.[8] The probability to pin a step in a given energy minimum is proportional to $\exp[(\Delta U - wf)/kT]$. This implies that the slope $\phi = d\zeta/dx \propto \exp[(\Delta U - wf)/kT]$. From this we can extract the healing length

$$x_0 = \frac{kT}{(\rho_\mathrm{s} - \rho_\mathrm{l}) g \tau a \ell w}, \tag{1}$$

where ℓ is the length of the jumping part of the step.

The main uncertainty in comparing this model with experiments is that both ℓ and w are poorly known. Anyway, we can estimate $x_0 \sim 1$ mm in agreement with experiment. Also, the dependence on temperature is roughly

right. A difficulty in the comparison arises because the data was originally analyzed in order to get the surface stiffness, and the raw data on x_0 was no more easily available. Thus only part of the data measured in Ref. 1 is used here. This consisted only of two values of tilting angle: $\tau = 0.0121$ and $\tau = 0.0045$ rad, and there was only one data point for the latter value. This one point is in disagreement with the τ dependence in Eq. (1). For a proper comparison a reanalysis of the data is needed.

The pinning of steps is also consistent with the observation that the angle ϕ on both sides of the discontinuity at the facet edge varies in an irreproducible fashion.

4. CONCLUSION

A simple model for the curving of facets was presented. It can account for most of the experimental observations. The major unsolved problem is the source of the pinning. Vacancies might be too mobile to act as pinning centers. Some alternatives are other point defects, edge or screw dislocations, ^{3}He impurities and surfaces of the experimental container.

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