On the transmission of crystallisation waves across the edge between the rough and faceted crystalline surfaces in superfluid $^4$He

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The wavelike processes of crystallisation and melting or crystallisation waves are well-known to exist at the crystal $^4$He surface in its rough state. Below the roughening transition temperature the crystal surface experiences the transition to the smooth faceted state and the crystallisation waves represent the propagation of a train of crystalline steps at the velocity depending on the crystal step height. Here we analyse the transmission and reflection of crystallisation waves propagating across the crystal edge separating the crystal surface in the rough and faceted states.

I. INTRODUCTION

Helium crystals as a model system can provide us with very general and unusual properties of liquid-solid interfaces [1, 2]. On one hand, helium crystals demonstrate faceting as classical crystals. The so-called roughening transition is the transition from the atomically rough and fluctuating state of the crystalline surface at high temperatures to the smooth faceted surfaces at sufficiently low temperatures. The experimental observations have displayed several roughening transitions in the hcp $^4$He crystals, as follows: $T_{R1}=1.3$ K for c-facet in the [0001] direction, $T_{R2}=1.07$ K for a-facet in the [1010] direction perpendicular to the c-axis, and $T_{R3}=0.36$ K for s-facet in the [1011] direction. The [1011] direction is tilted by 58.5° with respect to the [0001] direction.

On the other hand, as compared with classical crystals, the $^4$He crystals under ultralow energy dissipation can demonstrate the growth dynamics when quantum mechanics plays a major role [1, 2]. In particular, at sufficiently low temperatures the $^4$He crystal in contact with its superfluid phase can support oscillations of the superfluid-solid interface due to weakly damped processes of melting and crystallisation [3]. From the dynamical point of view such weakly damped crystallisation waves at the rough crystal surface are an immediate counterpart of the familiar gravitational-capillary waves at the interface between two normal liquids and have the similar dispersion as a function of wave vector.

On the contrary, no basic study of the melting-crystallisation dynamics has been made at the well-faceted and atomically smooth $^4$He crystal surfaces which, unlike the atomically rough crystal surfaces, have an infinitely large surface stiffness. Accordingly, the crystal surface curvature vanishes and the crystal facet takes the flat shape. The most striking distinction of smooth faceted crystal surfaces from the rough ones is the existence of non-analytical cusplike behaviour in the angle dependence of the surface tension, e.g. Ref. [4]. The crystal step energy becomes nonzero and positive below the roughening transition temperature $T_R$, vanishing at the higher temperatures. The origin of the singularity is directly connected with nonzero magnitude of the facet step energy below the roughening transition temperature.

As compared with the melting-crystallisation wave-like processes at the rough crystal surface, the analogous processes at the faceted crystal surface demonstrate a more complicated picture than those at the rough crystal surface [3]. The frequency spectrum of crystallisation waves at the faceted crystal surface has a sound-like dispersion with the velocity depending significantly on the wave perturbation amplitude and the number of facet steps distributed over the wavelength [3, 4]. In essence, such crystallisation waves represent a propagation of a train of crystal facet steps along the crystal surface at the velocity governed with the crystal step height. Here we mention the formation of crystallisation waves under heavy shake of an experimental cell [5] or in the process of anomalously fast growth of a $^4$He crystal under high overpressures [5, 6]. The progressive facet waves are observed at the crystal (001) facet in $^3$He [8].

The presence of singularity in the behaviour of surface tension or nonzero crystal step energy results also in a number of interesting phenomena at the facetted $^4$He crystal surface, e.g. amplitude-dependent velocity of traveling waves [5, 6], quantum fingering of the inverted liquid-crystal interface in the field of gravity [11], Rayleigh-Taylor instability with generating the crystallisation waves [12], and electrohydrodynamical instability [13] with breaking the faceted state down.

So far the crystallisation waves have been studied only for the spatially homogeneous crystalline surfaces. Since the adjacent crystal surfaces have the different roughening transition temperatures, we can raise a question about the propagation of melting-crystallisation waves across the edge between the crystal surfaces in the rough and smooth states. For the first time, in the present paper we attempt the transmission and reflection of crystallisation waves across the edge between the rough crystal surface and the smooth faceted surface of a $^4$He crystal.

II. LAGRANGIAN

The atomically rough surface and the atomically smooth surface of a $^4$He crystal correspond to various crystallographic directions and the surfaces contact each
other at the crystal edge. The transition from one direction to the other or from one surface to the other surface can be described with the polar angle which varies gradually from one value to another in order to parametrise two adjacent crystal surfaces.

In order to treat the transmission and reflection of crystallisation waves in most simplest and obvious way, we consider the following model situation. For simplicity, we assume that both the crystal surfaces, rough and smooth, are parallel to the $xy$ plane with the vertical position at $z = 0$. In addition, we imply that one-half of the crystal surface, e.g. $x < 0$, is in the rough state and the other half $x > 0$ is in the smooth facetted state. (Variable $x$ plays a role of polar angle.) First, we call $\zeta = \zeta(r)$ as a displacement of the crystal surface from its horizontal position $z = 0$ with $r = (x, y)$ as a two-dimensional vector. We neglect any anisotropy of the crystal surface in the $xy$ plane as well. We suppose sufficiently low temperature range in order to neglect any possible energy dissipation and the damping of crystallisation waves at the both states of the surfaces. This implies the temperatures lower than about 0.4 K. Neglecting the dissipation aspects simplifies mathematics as well.

As a result, in the lack of energy dissipation the surface oscillations of a $^4$He crystal can be described with the following Lagrangian:

$$L[\zeta(t, r), \dot{\zeta}(t, r)] = \frac{\rho_{\text{eff}}}{2} \int d^2r \int d^2r' \frac{\dot{\zeta}(t, r) \dot{\zeta}(t, r')}{2\pi |r - r'|} - \int d^2r \left( \alpha(\nu) \sqrt{1 + (\nabla \zeta)^2} + \frac{1}{2} \Delta \rho g \zeta^2 \right). \quad (1)$$

Here we ignore the compressibility of the both liquid and solid phases and $g$ is the acceleration of gravity. Because of low-temperature consideration we shall also neglect the normal component density in the superfluid phase or, equivalently, the difference between the superfluid density $\rho_s$ and the density of the liquid phase $\rho$, i.e. $\rho_s = \rho$. Then the effective interface density $\rho_{\text{eff}}$ is given by

$$\rho_{\text{eff}} = \frac{(\rho' - \rho)^2}{\rho} \approx 1.9 \text{ mg/cm}^3$$

and depends on the difference $\Delta \rho = \rho' - \rho$ between the solid density $\rho'$ and the liquid density $\rho$.

Unlike the fluid-fluid interface, the surface tension coefficient $\alpha(\nu)$ depends essentially on the direction of the normal $\nu$ to the interface against crystallographic axes. In our simplest description this is a function of the angle $\theta$ alone between the normal and, say, crystallographic [0001] or $c$ axis of the crystal hep structure with the geometric relation $|\tan \theta| = |\nabla \zeta|$. For the crystal facet tilted by small angle $\theta$ from the basal plane, the expansion of the surface tension $\alpha(\theta)$, usually written (see Refs. [1, 14]) as

$$\alpha(\theta) = (\alpha_0 + \alpha_1 \tan |\theta| + \ldots) \cos \theta, \quad |\tan \theta| = |\nabla \zeta|,$$

can be expanded for the small angles into a series

$$\alpha(\theta) = \alpha_0 + \alpha_1 |\theta| + \ldots, \quad |\theta| \ll 1.$$
III. TRANSMISSION AND REFLECTION

To consider the transmission and reflection of melting-crystallisation waves across the edge separating the rough surface and the crystal facet, we suppose a simple model to describe such phenomena. So, the step energy is approximated by the function

$$\alpha_1(x) = \begin{cases} 0, & x < 0 \\ \alpha_1, & x > 0. \end{cases}$$

In other words, the left-hand side of the crystal surface is in the rough state and the right-hand side of the crystal surface represents the smooth faceted state.

The approximation for step energy $\alpha_1(x)$ with the step-like function implies implicitly that the width of transition $W$ from the rough to smooth faceted state is much smaller as compared with the inverse wave vector $1/k$ or wavelength. The smooth boundary when $W \sim 1/k$ or larger should change the transmission and reflection coefficients. The smooth transition usually reduces the reflection and enhances the transmission of the wave.

As the crystallisation wave propagates across the boundary between two crystal surfaces, the wave transmits and reflects. The wave on the left-hand side of the boundary is a superposition of the incident and reflected waves. On the right-hand side from the boundary the transmitted wave alone propagates. The relation between all three waves is determined with the boundary condition that for the finite magnitude of the total surface energy.

We first neglect the gravitational term proportional to the density difference $\Delta \rho$ in the Lagrangian, assuming that wave vector is larger than the inverse magnitude of capillary length $k > k_0 \sim \sqrt{\Delta \rho / \alpha_0}$. Then, for the rough state of crystal surface, one has an ordinary capillary dispersion

$$\rho_{\text{eff}} \omega^2 = \alpha_0 k^2$$

and

$$k(\omega) = \left(\frac{\omega^2 \rho_{\text{eff}}}{\alpha_0}\right)^{1/3}.$$

For the faceted state of the crystal surface, the dispersion is more complicated and depends on the wave amplitude $\zeta$ according to

$$\rho_{\text{eff}} \omega^2 = \begin{cases} \gamma \alpha_1 q / |\zeta|, & |\zeta| \ll \alpha_1 / \alpha_0, \\
\alpha_0 q^2, & |\zeta| \gg \alpha_1 / \alpha_0, \end{cases}$$

where $\gamma = \pi \zeta(3)/7 = 0.539\ldots$ is a numerical coefficient. Accordingly,

$$q(\omega, \zeta) = \begin{cases} \omega \left(\frac{\rho_{\text{eff}} |\zeta|}{\gamma \alpha_1}\right)^{1/2}, & \omega^2 |\zeta|^3 \ll \frac{\alpha_1^3}{\alpha_0 \rho_{\text{eff}}}, \\
\omega \left(\frac{\rho_{\text{eff}} q}{\alpha_0}\right)^{1/3}, & \omega^2 |\zeta|^3 \gg \frac{\alpha_1^3}{\alpha_0 \rho_{\text{eff}}}. \end{cases}$$

The most interesting case is that of sufficiently small amplitudes $|\zeta_0|$ of the incident crystallisation wave satisfying the inequality $2k|\zeta_0| \ll (\alpha_1/\alpha_0)^{2/3} \lesssim 1$. The latter implies $q \ll k$. As a final result, we arrive at

$$\zeta_2 \approx 2\zeta_0, \quad \zeta_1 \approx \left(1 - \frac{2q}{k}\right)\zeta_0 \quad \text{and} \quad \frac{q}{k} \approx \sqrt{\frac{2\alpha_0}{\alpha_1}|\zeta_0|}.$$
Thus, we have approximately the following reflection and transmission coefficients: \( r \approx 1 \) and \( t \approx 2 \).

Let us discuss the result obtained. We see that the reflected crystallisation wave has approximately the same amplitude and is similar to the incident wave but propagating in the opposite direction. At the same time the incident wave onto the boundary edge induces the transmitted crystallisation wave with the double amplitude representing the flat kink at the smooth crystal surface. Such soliton-like perturbation, which size is about wavelength \( 2\pi/k \), propagates away from the boundary due to difference in the surface tension coefficients for the hand sides of the crystal surface. In its turn, the transmitted wave in the shape of a soliton with the larger wavelength.

In the opposite case of sufficiently large amplitudes, if \( 2k|\zeta_0| \gg (\alpha_1/\alpha_0)^{2/3} \), the reflected crystallisation wave is weak and practically vanishes since the facet step energy \( \alpha_1 \) plays a negligible role. The reflection can appear only due to difference in the surface tension coefficients for the adjoint crystal facets:

\[
r \approx \frac{\alpha_{0r}^{1/3} - \alpha_{0t}^{1/3}}{\alpha_{0r}^{1/3} + \alpha_{0t}^{1/3}},
\]

where coefficients \( \alpha_{0r} \) and \( \alpha_{0t} \) refer to the left- and right-hand sides of the crystal surface. In its turn, the transmitted crystallisation wave has an almost full similarity with the incident crystallisation wave. Thus, we expect \( r \approx 0 \) and \( t \approx 1 \) if \( \alpha_{0l} = \alpha_{0r} \).

IV. INCIDENCE FROM THE CRYSTAL FACET ONTO THE ROUGH CRYSTAL SURFACE

Let us consider the opposite situation when the crystallisation wave or crystal step arrives at the boundary from the smooth faceted surface to the rough crystal surface. So, we represent the incident, reflected and transmitted waves as follows:

\[
\zeta_0(x, t) = \zeta_0 e^{-iqx - i\omega t}, \quad x > 0,
\]

\[
\zeta_1(x, t) = \zeta_1 e^{iqx - i\omega t}, \quad x > 0,
\]

\[
\zeta_2(x, t) = \zeta_2 e^{-iqx - i\omega t}, \quad x < 0.
\]

Then, we have the following conditions at the boundary \( x = 0 \):

\[
\zeta_0 + \zeta_1 = \zeta_2 \quad \text{and} \quad -iq\zeta_0 + iq\zeta_1 = -ik\zeta_2.
\]

Hence we arrive at

\[
\zeta_2 = \frac{2q(\omega, \zeta_0)}{q(\omega, \zeta_0) + k(\omega)}\zeta_0, \quad \text{and} \quad \zeta_1 = \zeta_0 - \zeta_2(\zeta_0).
\]

Again the most interesting case is when the amplitude of the incident wave is sufficiently small \( q|\zeta_0| \ll \alpha_1/\alpha_0 \ll 1 \). This means, either the crystal step height is small, or

the length of protrusive crystal layer is rather extended. So, we find that the wave vector of the transmitted wave is given by

\[
k = q(\omega)
\]

\[
\left( \frac{\gamma_0}{\alpha_0} \frac{1}{q(\omega)|\zeta_0|} \right)^{1/3} \gg q(\omega)
\]

and the reflection and transmission coefficients read

\[
r = \frac{\zeta_1}{\zeta_0} \approx 1 \quad \text{and} \quad t = \frac{\zeta_2}{\zeta_0} \approx 2 \left( \frac{\alpha_0}{\alpha_1} \right)^{1/3} \ll 1.
\]

Thus, we see that the crystallisation wave or the crystal step, on the whole, reflects from the rough crystal surface. As it concerns the transmitted wave, its amplitude is much smaller as compared with the amplitude of the incident wave and the excitation of the crystallisation wave at the rough surface with the incident crystal step is ineffective. Here we should underline some asymmetry between the incidence of crystallisation waves from the rough and from the faceted crystal surface sides.

In the opposite limit when \( q|\zeta_0| \gg \alpha_1/\alpha_0 \) the difference between the faceted state and the rough state is not large. We expect practically no reflection from the boundary and the full transmission of the wave to the other side of the crystal surface. In fact,

\[
k \approx q(\omega) + \frac{\gamma_0}{3\alpha_0 q|\zeta_0|}
\]

and the reflection and transmission coefficients are approximately given by

\[
r = \zeta_1 \approx \frac{1}{6} \frac{\gamma_0}{\alpha_0 q|\zeta_0|} \ll 1 \quad \text{and} \quad t = \frac{\zeta_2}{\zeta_0} \approx 1.
\]

The latter means that the noticeable reflection can again appear only due to large distinction in the surface tension coefficients of the left-hand and right-hand sides of a crystal.

V. SUMMARY

To conclude, for the first time we have attempted the transmission and reflection of crystallisation waves propagating in a \(^4\text{He}\) crystal across the boundary edge between the crystal surfaces in the rough and smooth states. The crystallisation wave at the rough \(^4\text{He}\) crystal surface resembles the usual gravitational-capillary waves at the fluid-fluid interface. In contrast, the crystallisation wave at the smooth faceted surface in essence represents the propagation of crystal steps at the velocity depending on the crystal step height. To match two types of waves at the crystal edge, we use the natural boundary conditions.

Since the dispersion of crystallisation waves at the smooth faceted surface is essentially governed with the wave amplitude, the transmission and reflection coefficients depend on the amplitude of the incident wave. The incidence of the crystallisation wave from the rough
crystal surface onto the smooth faceted one results in
the practically mirror reflection of the incident wave and
in inducing the crystal step or soliton of about double
amplitude in the region of the crystal facet behind the
crystal edge.

In the opposite situation of the incidence of the crys-
tallisation wave from the faceted crystal surface onto the
rough crystal surface we should observe practically the
full reflection and the corresponding small transmission
to the rough crystal surface. Note that we have no sym-
metry with respect to rearrangement between the crystal
surfaces in the rough and flat states.

The experimental study on the dynamics of crystallisation
waves at the atomically smooth crystal facet requires
an effective mechanism for their excitation. Apparently
this is a tough challenge. To confirm, we can mention an
unsuccessful attempt to produce a soliton-like crystallisa-
tion wave with the aid of a Π-shaped crossbar oscillating
in the vicinity of the crystal 4He facet [16]. The oscilla-
tions of the crossbar are shown to be very effective for
inducing the crystallisation waves at the rough 4He crys-
tal surface but no effect is observed for the faceted 4He
crystal surface.

The present work proposes a mechanism for exciting
the wave or soliton at the smooth flat facet with the help
of crystallisation wave propagating along the non-faceted
rough surface across the crystal edge in the direction to
the atomically smooth facet. One more possibility is to
prepare the electron-charged crystal facet in order to in-
duce the instability of the atomically smooth surface at
the critical electron density. However, this will require
the larger critical electron density [13] by a factor of
about 50 – 100 as compared with that of about 10^9 cm^{-2}
observed for the rough interface.

A special interest represents the experiment on the
transmission and reflection of crystallisation waves propa-
 gating across the crystal edge between the rough crystal
surface and the vicinal surface whose orientation is tilted
by the small angle θ with respect to the well-faceted
surface. Provided the tilt angle θ is sufficiently small,
the crystal steps are well separated. On the other hand,
an existence of ready-made crystal steps should notice-
ablely affect the transmission and reflection coefficients as
a function of tilt angle of the vicinal surface. We hope an
experimental production and examination of soliton-like
crystallisation waves at the crystal 4He facet below the
roughening transition temperature would be fascinating
and incredible.

Acknowledgments

The present study is performed with the pleasant col-
laboration with V.L. Tsymbalenko. The author is also
grateful to L.B. Dubovskii.

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