Two-velocity elasticity theory and facet growth

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Abstract

We explain the linear growth of smooth solid helium facets by the presence of lattice point defects. To implement this task, the framework of very general two-velocity elasticity theory equations is developed. Boundary conditions for these equations for various surface types are derived. We also suggest additional experiments to justify the concept.

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1 Introduction

Existence of two distinct states of a crystal surface is well known: it may be either smooth or rough (for a review, see [1]). A smooth surface is characterized by a long-range order and small fluctuations. On the contrary, a rough surface behaves differently — it does not exhibit a long-range order and its displacement fluctuates heavily. These equilibrium properties lead to different kinetic properties. While the rough surface is usually supposed to grow easily (as described by the growth coefficient), the smooth one (providing the crystal has no dislocations) is characterized by zero growth coefficient and grows with nuclei of new atomic layer. In accordance with this mechanism, one should not observe the linear growth rate if low overpressure is applied. Reality is different — experiments [2] demonstrate that a smooth helium surface free of screw dislocations grows linearly. This work is an attempt to explain this behavior by the presence of lattice point defects (vacancies). The idea is similar to that suggested by Herring [3] and by Lifshitz [4] as an explanation of polycrystal flow. It is quite simple: the mass flux in bulk helium is attributed to the motion of vacancies. This flux is the mass transfer through the lattice. Therefore, if vacancies are allowed to be created on the bottom edge of the sample (the boundary between the crystal and the wall, see Fig. 1) and to annihilate on the top of it (on the smooth crystal-liquid interface), then the crystal grows.

Figure 1: Typical experimental layout

The suggested crystal growth mechanism may be explained as follows. Since the smooth crystal facet (the top one in Fig. 1) cannot move with respect to the lattice, it moves upward stuck to the lattice. Vacuities to appear due to this on the bottom edge of the crystal transform into lattice defects (ordinary vacancies) and go up through (and faster than) the bulk helium. They finally vanish in the liquid on the top smooth
surface of the sample. In other words, the crystal grows on the boundary between helium and the wall, rather than on the smooth solid-liquid interface (which nevertheless provides mass supply for the growth). It is important to emphasize that this scenario may occur if and only if the vacancies are allowed to emerge on the bottom edge of the crystal. One may say that this boundary is in some sense “atomically rough” — it can grow new atomic layers. For this condition to be satisfied, the wall surface should have a disordered shape or be slightly tilted with respect to basal planes of the crystal (thereby forming a vicinal interface). This ensures that the surface can play the role of a source or a sink of vacancies. An atomically flat wall parallel to the basal plane should, in contrast, behave like a normal smooth surface — it is fixed to the lattice. This is due to the fact that for the surface to move new atomic layer nuclei have to be created.

This paper is organized as follows. In Secs. 3 and 5 we derive very general two-velocity elasticity theory equations. They consist of conditions for the conventional elasticity theory variables (including lattice velocity) and equations for a macroscopic description of the quasiparticle gas (including the quasiparticle gas velocity).

Equations to be derived are similar to those of the two-velocity superfluid hydrodynamics. Velocities of lattice and excitation gas in our equations replace superfluid and normal component velocities of the two-fluid hydrodynamics. Similarly to the usual linear phonon hydrodynamics (see § 71) Umklapp-process (which result in the nonconservation of the total quasimomentum in quasiparticle collisions) probability is supposed to be low. In the low-temperature region considered here this assumption is quite reasonable. We also neglect dissipation here. This means that our analysis is limited to the terms of the first order in gradients.

Derivation procedure of exact (nonlinear) hydrodynamics equations for superfluid can be implemented (see § 6) from phenomenological considerations, using conservation laws. A constitutive argument for this derivation is the statement that the superfluid flow is potential. This is an intrinsic property of the order parameter in a superfluid. Such condition is unavailable for a crystal (moreover, there is no quasimomentum conservation relation in the nonlinear description, see Eq. (13) below).

We deduce the two-velocity elasticity theory equations using a more general approach (see the paper by Pushkarov and one of the authors [7], as well as [8] and [9]). It is based on the kinetic equation description of the quasiparticle dynamics. The realization of this technique, particularly in nonlinear situation, is a matter of considerable interest for its own sake not only for a solid but also for a superfluid (that this procedure is possible is mentioned in § 71). With this technique, we find exact expressions for all hydrodynamic variables and their dependence (in terms of the quasiparticle energy spectrum) on the relative velocity of components. It is trivial to extend the equations obtained for the solid dynamics to the simpler case of superfluid hydrodynamics.

Boundary conditions for our equations depend on the surface type; in Sec. 5 we thoroughly consider three possibilities: rough (Sec. 4.1.1) and smooth (Sec. 4.1.2) interfaces between solid and liquid helium, and the rough boundary between solid helium and normal hard wall (Sec. 4.2.1). Finally, in Sec. 5 we calculate the growth rate for the crystal.

2 Definitions

Following the principles in Refs. [7, 8, 9] we employ the Euler approach to the lattice description. We thus introduce three “node numbers” $N^\alpha$ ($\alpha = 1, 2, 3$). They are functions of space coordinates $r$ and time $t$, $N^\alpha = N^\alpha(r, t)$. From now on, Greek indices (like $\alpha$ here) are used for the “lattice space” and Latin indices (e.g., $i$ in $x_i$ for the components of $r$) for the real space components. Defining the reciprocal lattice vectors as $a^\alpha = \partial N^\alpha/\partial r$, we get the elementary lattice translation vectors $a_\beta$ as $a^\alpha a_\beta = \delta_\beta^\alpha$. Taking the time derivative, we obtain the lattice velocity as $w = -a_\alpha N^\alpha$. The elastic energy $E_l$ of the lattice is a function of the deformation. Moreover, since it depends not on the spatial orientation of the infinitesimal sample (the space is isotropic), but on the relative position of the $a^\alpha$ vectors, we may write $E_l = E_l(g^{\alpha\beta})$, where $g^{\alpha\beta} = a^\alpha a^\beta$ is a symmetric “metric tensor” of the lattice space.

We are now ready to describe quasiparticle degrees of freedom. We do not specify the quasiparticle nature at the moment (be it phonons, vacancies as in [7], or electrons as in [9]). Actually, all the equations below imply the summation over all branches of excitations; we do not explicitly write the sum for brevity. Any quasiparticle should be characterized by its mass $m$ (zero for phonons, positive for electrons, and negative for vacancies), coordinate, and momentum. Since quasiparticles exist in the lattice background, the quasimomentum should be used. Their energy in the frame of reference of the lattice $\epsilon = \epsilon(a_\alpha(p - m w), g^{\alpha\beta})$
is a periodic function of the quasimomentum $\mathbf{p}$ (its periods are $2\pi \hbar \mathbf{a}^\beta$). In laboratory frame of reference, we have the quasiparticle energy (see [3])

$$\tilde{\epsilon} = \epsilon + m \mathbf{w} \frac{\partial \epsilon}{\partial \mathbf{p}} + m \frac{w^2}{2}.$$  

We also use the variables $\mathbf{k} = \mathbf{p} - m \mathbf{w}$ and $k_\alpha = a_\alpha \mathbf{k}$. Quasiparticle dynamics is determined by the Hamilton function

$$H = \epsilon + \mathbf{p} \mathbf{w} - m \frac{w^2}{2}.$$  

We now introduce the distribution function $f(\mathbf{r}, \mathbf{p})$ (it is also a periodic function of the quasimomentum $\mathbf{p}$).

Its kinetics is governed by the Boltzmann equation

$$\frac{\partial f}{\partial t} + \frac{\partial f}{\partial \mathbf{r}} \frac{\partial H}{\partial \mathbf{p}} - \frac{\partial f}{\partial \mathbf{p}} \frac{\partial H}{\partial \mathbf{r}} = S f.$$  

Using this distribution function, we can obtain macroscopic quantities like the mass density as

$$\rho = \rho_l + \langle mf \rangle = M \det (g^{\alpha \beta})^{1/2} + mn,$$

where the angle brackets denote the integration over quasimomentum space, $\langle \rangle = \int \frac{d^3 p}{(2\pi \hbar)^3}$, $\rho_l$ is the lattice density, $M$ is the mass of an elementary cell, and $n = \langle f \rangle$.

We consider a quasi-equilibrium distribution function. The complete set of quantities conserved in quasiparticle collisions consists of their mass (proportional to their quantity for "real" particles like electrons and vacancies and zero for phonons), energy, and quasimomentum (in the low-temperature region, Umklapp processes may be neglected). Consequently, the most general quasi-equilibrium distribution is a function of

$$z = \frac{\epsilon - \mathbf{kv} - m \mu_0}{T} = \frac{\epsilon - (\mathbf{p} - m \mathbf{w}) \mathbf{v} - m \mu_0}{T} = \frac{\epsilon - \mathbf{p} \mathbf{v} - m \mu_0 + m \mathbf{w} \mathbf{v}}{T} = \frac{\epsilon - \mathbf{p} \mathbf{v} - m \phi}{T},$$

where $\mu_0 - \mathbf{w} \mathbf{v} = \phi$. The Lagrange coefficients $T$, $\mathbf{v}$, and $\mu_0$ denote temperature, the velocity relative to the lattice, and chemical potential of the quasiparticle gas, accordingly. For definiteness, we assume that the excitations are Bose particles. The distribution function is then given by

$$f = \frac{1}{e^z - 1} = \left( \exp \frac{\epsilon - \mathbf{p} \mathbf{v} - m \phi}{T} - 1 \right)^{-1},$$

and $\ln((f + 1)/f) = z$.

We can now calculate other macroscopic parameters with this distribution function. For the mass flux, we have

$$\mathbf{J} = \rho_l \mathbf{w} + \mathbf{w} mn + \mathbf{j} = \rho \mathbf{w} + \mathbf{j} = \rho \mathbf{w} + mn \mathbf{v},$$

where the mass flux with reference to the lattice is

$$\mathbf{j} = m \left\langle f \frac{\partial \epsilon}{\partial \mathbf{p}} \right\rangle = mn \mathbf{v}.$$  

Using $\mathbf{J}$, we can write the mass conservation as

$$\dot{\rho} + \mathbf{J}_i, i = 0.$$  

The number of real (massive) particles is also conserved in the bulk, and we therefore have one additional conservation law

$$\dot{\rho}_l + (\rho_l w_i)_i, i = 0.$$  

\footnote{For further convenience, we also provide here the result of the distribution function integration:

$$\int f \, dz = \ln \frac{e^z - 1}{e^z} = -ln(f + 1).$$}
Similarly, the energy density is given by

\[ E = \rho_1 \frac{w^2}{2} + E_i (g^{\alpha \beta}) + \langle \epsilon f \rangle = \rho \frac{w^2}{2} + \mathcal{E}_i (g^{\alpha \beta}) + \mathbf{w} \cdot \mathbf{j} + \langle \epsilon f \rangle. \]  

This equation allows us to prove (and find) exact macroscopic equivalents of the microscopic quantities introduced above. The total energy density of the crystal can be obtained via a Galilean transformation,

\[ E = E_0 + \frac{\rho w^2}{2} + \mathbf{j} \mathbf{w}, \]

where \( E_0 = E_0 (a^\alpha, S, \rho, \mathbf{K}) \) is the energy in the frame of reference of the lattice, with \( \mathbf{K} = \langle \mathbf{k} \rangle \) characterizing the quasimomentum density. A reasonable expression for the \( E_0 \) differential

\[ dE_0 = \lambda_{ij} a_{ij} + T dS + \mu d\rho + \mathbf{v} d\mathbf{K} \]

we obtain with the conventional definition of the entropy density for the Bose gas,

\[ S = \langle (f + 1) \ln (f + 1) - f \ln f \rangle = \langle f x + g f \rangle. \]

Its differential being

\[ dS = \langle (\ln (f + 1) + 1 - \ln f - 1) d\mathbf{f} \rangle = \langle z d\mathbf{f} \rangle. \]

Subtracting the differentials of (4) and (5), we obtain

\[ 0 = \lambda_{ij} a_{ij} + T dS + \mu d\rho + \mathbf{v} d\mathbf{K} - dE_i (g^{\alpha \beta}) - \langle \epsilon f \rangle \]

\[ = \lambda_{ij} a_{ij} + T \langle z d\mathbf{f} \rangle + \mu d\rho + \mathbf{v} d\mathbf{K} - dE_i (g^{\alpha \beta}) - \langle \epsilon f \rangle - \langle f d\mathbf{e} \rangle \]

\[ \lambda_{ij} a_{ij} + \langle (T z + \mathbf{v} \mathbf{k}) d\mathbf{f} \rangle + \mu d\rho - dE_i (g^{\alpha \beta}) + \mathbf{v} \langle f d\mathbf{k} \rangle - \langle f d\mathbf{e} \rangle \]  

We now transform the part of this equation related to the lattice deformation

\[ \frac{\mu}{2} \rho g_{ab} d\mathbf{g}^{ab} - dE_i (g^{\alpha \beta}) + \mathbf{v} \langle f d\mathbf{k} \rangle - \langle f d\mathbf{e} \rangle = \frac{\mu}{2} \rho g_{ab} d\mathbf{g}^{ab} - \frac{\partial E_i}{\partial g^{ab}} d\mathbf{g}^{ab} - mv \langle f d\mathbf{w} \rangle \]

\[ - \left\langle f \left( \frac{\partial \epsilon}{\partial \mathbf{k}_a} ((\mathbf{p} - m\mathbf{w}) \mathbf{a}_a - m \mathbf{a}_a d\mathbf{w}) + \left( \frac{\partial \epsilon}{\partial g^{ab}} \right)_{\mathbf{k}_a} d\mathbf{g}^{ab} \right) \right\rangle \]

\[ = - \left( \frac{\partial E_i}{\partial g^{ab}} + \left\langle f \left( \frac{\partial \epsilon}{\partial g^{ab}} \right)_{\mathbf{k}_a} \right\rangle \right) d\mathbf{g}^{ab} + \left( \mu \rho \delta_{ij} - \left\langle f \left( \frac{\partial \mathbf{g} \cdot \mathbf{v}}{\partial p_j} (p_i - m w_i) \right) a^\alpha_{ij} \right\rangle \right) d\mathbf{a}_i \]

\[ = - \left( \frac{\partial E_i}{\partial g^{ab}} + \left\langle f \left( \frac{\partial \epsilon}{\partial g^{ab}} \right)_{\mathbf{k}_a} \right\rangle \right) 2a^\alpha_{ij} a^\beta_{ij} d\mathbf{a}^\nu \]

\[ + \left( \delta_{ij} (T \langle \ln (f + 1) \rangle + \mu \mathbf{P}_f) + v_i \mathbf{P}_j - m\mathbf{v} \cdot \mathbf{w}_j \right) a_{ij} \]

\[ = \left( \delta_{ij} \left( TS + \rho \frac{w^2}{2} + E_i - E + \mathbf{P} \mathbf{v} + \mu \rho t + m \mu_0 \right) - \lambda_{ij} + v_i \mathbf{P}_j - m\mathbf{v} \cdot \mathbf{w}_j \right) a_{ij}. \]

Finally, from (7) we get:

\[ 0 = (\mu - \mu_0) m d\mathbf{n} \]

\[ + \left\{ \lambda_{ij} - \Lambda_{ij} + \delta_{ij} \left( TS + E_i - E + \mu \rho + \mathbf{P} \mathbf{v} + \rho \frac{w^2}{2} \right) + v_i \mathbf{P}_j - m\mathbf{v} \cdot \mathbf{w}_j \right\} a_{ij} d\mathbf{a}^\nu, \]

where we introduced \( P_i = \langle p_i \rangle \) and

\[ \Lambda_{ij} = 2a^\alpha_{ij} a^\beta_{ij} \left( \frac{\partial E_i}{\partial g^{ab}} + \left\langle f \left( \frac{\partial \epsilon}{\partial g^{ab}} \right)_{\mathbf{k}_a} \right\rangle \right). \]

The terms in (8) are independent, and each of them must therefore be equal to zero. That is,

\[ \mu = \mu_0, \]

\[ \lambda_{ij} = \Lambda_{ij} - \delta_{ij} \left( TS + E_i - E + \mu \rho + \mathbf{P} \mathbf{v} + \rho \frac{w^2}{2} \right) - \Lambda_{ij} + v_i \mathbf{P}_j + m\mathbf{v} \cdot \mathbf{w}_j. \]
3 Equations and Fluxes

Here, we derive dynamics equations and thermodynamic fluxes for the system. Neglecting dissipation at this point, we assume that the entropy conservation law is valid,

$$\dot{S} + F_{i,i} = 0,$$

where the entropy flux $F_i$ is determined by

$$F_i = S(v + w).$$

We continue with the equation for the momentum flux found in [2],

$$\dot{J}_i + \Pi_{i,k,k} = 0,$$

where

$$\Pi_{i,k} = \rho w_i w_k - E_i \delta_{i,k} + 2 \alpha_i \alpha_k \left( \frac{\partial E_i}{\partial \alpha_i} + \left( f \left( \frac{\partial \epsilon}{\partial \alpha_i} \right) \right) \right) + w_{i,j} + w_{k,j},$$

$$= \rho w_i w_k - E_i \delta_{i,k} + mn(w_i v_k + w_k v_i) + 2 \alpha_i \alpha_k \left( \frac{\partial E_i}{\partial \alpha_i} + \left( f \left( \frac{\partial \epsilon}{\partial \alpha_i} \right) \right) \right)$$

$$= \rho w_i w_k - E_i \delta_{i,k} + mn(w_i v_k + w_k v_i) + \Lambda_{i,k},$$

where we employed the definition [3] for $\Lambda_{i,k}$.

Taking the appropriate equation for the energy flux from [7], we have

$$\dot{E} + Q_{i,i} = 0,$$

where

$$Q_i = w_i E_i + \left\langle \frac{\partial H}{\partial p_i} f \right\rangle - \frac{w_i^2}{2} J_i + w_k \Pi_{i,k}.$$ 

To find the second term, we again use the distribution function from [2],

$$\left\langle \epsilon \frac{\partial H}{\partial p_i} f \right\rangle = \left\langle \epsilon \left( \frac{\partial \epsilon}{\partial p_i} + w \right) f \right\rangle$$

$$= \left\langle \epsilon \left( T \frac{\partial z}{\partial p_i} + v_i + w_i \right) f \right\rangle = (v_i + w_i) \langle \epsilon f \rangle + T \left\langle (T x + \rho v + \phi) \frac{\partial z}{\partial p_i} f \right\rangle$$

$$= (v_i + w_i) \langle \epsilon f \rangle - T \left\langle \rho v \frac{\partial \ln(1 + f)}{\partial p_i} \right\rangle = (v_i + w_i) \langle \epsilon f \rangle + T v_i \langle \ln(1 + f) \rangle$$

$$= (v_i + w_i) \langle \epsilon f \rangle + T v_i \langle \ln(1 + f) + f \ln \left( \frac{f + 1}{f} \right) \rangle - T v_i \left\langle \frac{\epsilon - \rho v - m\phi}{T} \right\rangle$$

$$= (v_i + w_i) \langle \epsilon f \rangle + T v_i S - v_i \langle f \epsilon \rangle + v_i v_P + mn \phi = w_i \langle \epsilon f \rangle + v_i (T S + v_P + mn \phi).$$

For the energy flux, we finally have

$$Q_i = w_i \langle \epsilon f \rangle + v_i (T S + v_P + mn \phi) - \frac{w_i^2}{2} \rho w_i w_k + mn(w_i v_k + w_k v_i) + \Lambda_{i,k}$$

$$= w_i \langle \epsilon f \rangle + v_i (T S + v_P + mn \phi) + \frac{w_i^2}{2} \rho w_i w_k + mn(w_i v_k + w_k v_i) + \Lambda_{i,k}$$

$$= w_i \left( \langle \epsilon f \rangle + \rho \frac{w_i^2}{2} \right) + v_i \left( T S + v_P + mn \phi + \frac{w_i^2}{2} \right) + w_k \Lambda_{i,k}$$

$$= v_i \left( T S + v_P + mn \phi + \frac{w_i^2}{2} \right) + w_i (E - E_i) + w_k \Lambda_{i,k}. \quad (14)$$

This formula completes the list of the conventional elasticity theory equations. An additional equation is required to govern the quasiparticle degrees of freedom. We now find the time derivative of $P_i$. We multiply
Boltzmann equation \( \mathbf{p} \) by \( \mathbf{p}_i \) and integrate over the momentum space. We temporarily neglect Umklapp processes, which are supposedly rare. If needed, dissipation can be explicitly introduced into the final result. In other words, the quasimomentum \( \mathbf{p} \) is conserved in (normal) collisions, and the term involving the collision integral is therefore zero. The left-hand side of the Boltzmann equation gives

\[
\dot{P}_i = \left< p_i \left( \frac{\partial f}{\partial \mathbf{p}} \frac{\partial H}{\partial \mathbf{r}} - \frac{\partial f}{\partial \mathbf{r}} \frac{\partial H}{\partial \mathbf{p}} \right) \right> = \left< p_i \left( \frac{\partial f}{\partial \mathbf{p}} \frac{\partial \mathbf{r}}{\partial \mathbf{r}} + (p_j - m w_j) \frac{\partial w_j}{\partial \mathbf{r}} - \frac{\partial f}{\partial \mathbf{r}} \left( \frac{\partial \mathbf{r}}{\partial \mathbf{p}} + \mathbf{w} \right) \right) \right>
\]

\[
= -f \left( \frac{\partial \mathbf{r}}{\partial x_i} + (p - m \mathbf{w}) \frac{\partial \mathbf{w}}{\partial x_i} \right) - f p_i \left( \frac{\partial^2 \mathbf{r}}{\partial \mathbf{r}^2} + \frac{\partial \mathbf{w}}{\partial \mathbf{r}} \right) - p_i \frac{\partial f}{\partial \mathbf{r}} \frac{\partial \mathbf{r}}{\partial \mathbf{p}} - p_i \frac{\partial f}{\partial \mathbf{r}} \mathbf{w}
\]

\[
= - \left< f \frac{\partial \mathbf{r}}{\partial x_i} + f p_i \frac{\partial^2 \mathbf{r}}{\partial \mathbf{r}^2} + p_i \frac{\partial f}{\partial \mathbf{r}} \mathbf{r} + f \mathbf{w} \right> + \left< f \mathbf{w} \right> \frac{\partial \mathbf{r}}{\partial \mathbf{p}} + f \mathbf{w} + f \mathbf{w} \mathbf{w} \frac{\partial \mathbf{r}}{\partial \mathbf{p}} - \left< f \mathbf{w} \right> \mathbf{w}.
\]

The first term can be transformed as

\[
\left< f \frac{\partial \mathbf{r}}{\partial x_i} + f p_i \frac{\partial^2 \mathbf{r}}{\partial \mathbf{r}^2} + p_i \frac{\partial f}{\partial \mathbf{r}} \mathbf{r} + f \mathbf{w} \right> = \left< f p_i \frac{\partial^2 \mathbf{r}}{\partial \mathbf{r}^2} + f \mathbf{w} \right> \frac{\partial \mathbf{r}}{\partial \mathbf{r}} \left( T \frac{\partial \mathbf{z}}{\partial \mathbf{p}} + \mathbf{v} \right)
\]

\[
= \left< p_i \frac{\partial^2 \mathbf{r}}{\partial \mathbf{r}^2} + p_i \frac{\partial f}{\partial \mathbf{r}} \mathbf{r} + f \mathbf{w} \right> \frac{\partial \mathbf{r}}{\partial \mathbf{r}} \left( T \frac{\partial \mathbf{z}}{\partial \mathbf{p}} + \mathbf{v} \right) + \left< f \mathbf{w} \right> \frac{\partial \mathbf{r}}{\partial \mathbf{r}} \left( T \frac{\partial \mathbf{z}}{\partial \mathbf{p}} + \mathbf{v} \right)
\]

\[
= n m \frac{\partial \phi}{\partial x_i} + P \frac{\partial \mathbf{v}}{\partial x_i} + \frac{\partial}{\partial \mathbf{r}} (P \mathbf{v}) + \left< f \mathbf{w} \frac{1}{f} \ln(f + 1) \right> \frac{\partial \mathbf{r}}{\partial x_i}
\]

\[
= n m \frac{\partial \phi}{\partial x_i} + P \frac{\partial \mathbf{v}}{\partial x_i} + \frac{\partial}{\partial \mathbf{r}} (P \mathbf{v}) + \left< f \mathbf{w} \frac{1}{f} \ln(f + 1) \right> \frac{\partial \mathbf{r}}{\partial x_i}
\]

Consequently,

\[
\dot{P}_i = n m w \frac{\partial \mathbf{w}}{\partial x_i} - P \frac{\partial \mathbf{w}}{\partial x_i} - \frac{\partial}{\partial \mathbf{r}} (P \mathbf{w}) - n m \frac{\partial \phi}{\partial x_i} - P \frac{\partial \mathbf{v}}{\partial x_i} - \frac{\partial}{\partial \mathbf{r}} (P \mathbf{v}) - S \frac{\partial \mathbf{r}}{\partial x_i}
\]

\[
= n m \frac{\partial \phi}{\partial x_i} + \frac{\partial}{\partial \mathbf{r}} (P \mathbf{v}) + \frac{\partial}{\partial \mathbf{r}} (P \mathbf{w} + S \frac{\partial \mathbf{r}}{\partial x_i}) (15)
\]

The desirable complete set of the two-velocity elasticity theory equations consists of Eqs. (13), (13) (with \( Q \) defined by (14)), and (1) (with \( \Pi_{ij} \) defined by (12)).

4 Boundary Conditions

We now turn to boundary conditions. They immediately follow from the conservation relations to be satisfied at the interface. It is much easier to perform all transformations in the frame of reference of the interface itself. All the velocities are therefore taken relative to the boundary. Moreover, we simplify the problem by restricting it to the one-dimensional case: all fluxes are supposed to be perpendicular to the flat surface; we let the \( z \) axis run along this direction. Since no curvature is ascribed to the surface, we ignore capillary effects. All calculations done here are valid within the linear approximation. Naturally, boundary conditions should depend on the type of the boundary and on the type of the media on the other side of the interface. We begin with the situation extensively discussed in literature, the solid–liquid interface [1]. Because the possibility of the mass flux through the lattice is taken into account, the results are different, however.
4.1 Solid–Liquid Interface

The liquid on the other side of the interface (being superfluid) is characterized by the chemical potential $\mu^L$, normal and superfluid densities $\rho^S_n$ and $\rho^S_s$, normal and superfluid velocities $v^S_n$ and $v^S_s$, temperature $T^L$, pressure $p^L$, and the entropy density $S^L$ (see Fig. 2).

$$
\begin{align*}
R + S^L (v^S + w^S) &= S^L v^L_n, \\
w^S (E^S - E^L_i + \Lambda^S_{zz}) + w^S (T^S S^S + m^S n^S \phi^S) &= \mu^L (\rho^L_s v^L_s + \rho^L_n v^L_n) + S^L T^L v^L_n, \\
v^S m^S n^S + \rho^S w^S &= \rho^L_s v^L_s + \rho^L_n v^L_n, \\
\Lambda^S_{zz} - E^L_i &= p^L.
\end{align*}
$$

The superscript $S$ indicates that the appropriate quantities refer to the solid. The first equation is the entropy growth condition, where $R$ is the surface dissipative function. The last three equations in (16) are simply the requirements for the energy, mass, and momentum conservation for the surface, respectively. The surface dissipative function must be a positive square form. Using (16) and (17), it can be expressed as

$$
RT^L = v^S (S^S (T^S - T^L) + m^S n^S (\phi^S - \mu^L)) + w^S (E^S - E^L_i + \Lambda^S_{zz} - \rho^S \mu^L - T^L S^S) \\
= v^S (m^S n^S (\phi^S - \mu^L) + S^S (T^S - T^L)) + w^S (\Lambda^S_{zz} + \rho^S (\phi^S - \mu^L) + S^S (T^S - T^L)).
$$

We now recall that the solid–liquid boundary can be either atomically-rough or atomically-smooth, depending on the temperature. The nature of the surface may (or may not) impose certain restrictions on the dynamics. For both types of the surface, the equation

$$
\Lambda^S_{zz} - E^L_i = p^L
$$

is satisfied.

4.1.1 Rough Surface

Employing the Onsager principle, we obtain

$$
\begin{align*}
v^S &= \alpha (m^S n^S (\phi^S - \mu^L) + S^S (T^S - T^L)) + \eta (\Lambda^S_{zz} + \rho^S (\phi^S - \mu^L) + S^S (T^S - T^L)) \\
w^S &= \eta (m^S n^S (\phi^S - \mu^L) + S^S (T^S - T^L)) + \nu (\Lambda^S_{zz} + \rho^S (\phi^S - \mu^L) + S^S (T^S - T^L)).
\end{align*}
$$

The kinetic matrix $\begin{pmatrix} \alpha & \eta \\ \eta & \nu \end{pmatrix}$ is positively definite.

4.1.2 Smooth Surface

A smooth surface implies immobility of the interface relative to the lattice. That is,

$$w^S = 0.$$

Figure 2: Solid–liquid boundary: fluxes in one dimension
For the quasiparticle gas velocity, we then obtain a restricted version of [18],

\[ v^S = \alpha \left( m^S n^S (\phi^S - \mu^L) + S^S (T^S - T^L) \right), \]

(19)

with the kinetic coefficient \( \alpha > 0 \).

### 4.2 Solid–Wall Boundary

![Figure 3: Solid–wall boundary: fluxes in one dimension](image)

By a wall, we imply a macroscopically flat structureless medium, in short, “concrete”. The “Solid–wall” boundary occurs between solid helium and some normal rigid solid (silica in experiment [2]). A “concrete” wall is characterized by no mass flux in it (i.e., through the interface). The wall can supply an arbitrary energy flux; we let \( Q \) denote the flux and \( T^W \) the wall temperature (see Fig. 3). Concrete is characterized by fewer variables than liquid, and the appropriate equations are therefore somewhat simpler.

Just like for the solid–liquid interface, the actual boundary conditions must depend on the microscopic pattern of the surface. One can easily imagine a smooth basal plane of the crystal adjacent to an atomically flat concrete wall. This plane must stay at rest with respect to the wall since its motion presupposes the creation of new atomic layer nuclei. The plane is similar to the smooth solid–liquid interface, and we can naturally say that such an interface is smooth. The boundary condition is then given by \( w^S = v^S = 0 \).

Another, much more interesting scenario is realized if the interface is slightly tilted with respect to the basal plane. Such planes may move by growing additional nodes at the edge. This means that no restrictions are imposed on the lattice velocity near the interface. In other words, vacancies are allowed to freely appear and vanish on the surface (in this sense, the surface is similar to a grid of dislocations arranged at the boundary of the crystal that serve as sources or sinks for vacancies; similar speculations may be found in [4] in explaining polycrystal plasticity). We call this type of the interface “rough”. In this sense, the solid–wall boundary can be either smooth or rough. The suggested growth mechanism can be applied only to the rough boundary.

#### 4.2.1 Rough Boundary

Assuming the boundary to be rough and using the same approach as for the liquid, we write the conservation laws

\[
\begin{align*}
 w^S (E^S - E_i^S + \Lambda_{zz}^S) + v^S (T^S S^S + m^S n^S \phi^S) &= Q, \\
 v^S m^S n^S + \rho^S w^S &= 0.
\end{align*}
\]
Again, $R$ is the surface dissipative function,

$$RT^W = v^S \left( \frac{m^S n^S}{\rho^S} (E^S - E^S_l + \lambda^S_{zz} - \rho^S \phi^S - T^W S^S) + S^S (T^W - T^S) \right)$$

$$= v^S \left( \frac{m^S n^S}{\rho^S} \lambda^S_{zz} + \left( 1 - \frac{m^S n^S}{\rho^S} \right) S^S (T^W - T^S) \right).$$

It must be positive, and for the quasiparticle velocity on the surface we therefore have

$$v^S = \beta \left( \frac{m^S n^S}{\rho^S} \lambda^S_{zz} + \left( 1 - \frac{m^S n^S}{\rho^S} \right) S^S (T^W - T^S) \right),$$

where $\beta > 0$ is the surface kinetic coefficient.

## 5 The Growth Rate

We now use the equations and boundary conditions obtained above. The physical system discussed in what follows is solid helium with elementary excitations represented by phonons and vacancies. We first introduce a certain amount of friction between the quasiparticle gas and the lattice. To obtain a physically sound result, we again restrict our analysis to one dimension. Furthermore, for simplicity, all our calculations are performed within the linear approximation. We can write the quasimomentum density (with the superscript $S$ omitted) as $K = \rho_K v$, where

$$\rho_K \sim \frac{\hbar}{a^4 \Theta_D c}. \quad (21)$$

Here, $\Theta_D$ is the Debye temperature, $c$ is the velocity of sound in the crystal, and $a$ is the lattice period. The last equation is quite obvious. It follows from the fact that in the low-temperature region, the quasimomentum is mainly associated with phonons (the number of vacancies is exponentially small). The result therefore coincides with the one for the mass density (and the momentum density) of the normal component of the superfluid, $\rho_K \sim \rho_n \sim T^4/\hbar^3 c^3$ (see [10]).

![Figure 4: Crystal growth in one dimension](image)

To describe (rare) Umklapp events, we introduce the appropriate relaxation time parameter $\tau_U$. It is a "between-Umklapp-collision time". From (13), we then have

$$0 = \dot{K} = -mn \nabla \phi - S \nabla T - \frac{K}{\tau_U} = -mn \nabla \phi - S \nabla T - \rho_K \frac{v}{\tau_U}.$$
It is worth mentioning that \( \tau_U \) may well depend on both phonons and vacancies, despite the fact that the population of vacancies is far lower than that of phonons. For instance, if the vacancy energy band is sufficiently narrow, then the probability of Umklapp processes is significantly higher for vacancies than for phonons. This might overcome the low concentration of vacancies.

Interestingly enough, these formulas allow us to obtain the growth rate for a smooth surface. The quasiparticles playing the crucial role here (that of mass carriers) are vacancies, with their mass given by \( m = -m \nu \).

To estimate the rate, we write the temperature gradient as \( \nabla T = (T_2 - T_1)/h \), where the subscripts 1 and 2 stand for the solid–wall and the solid–liquid interfaces respectively (see Fig. 4). Likewise, for the chemical potential we write \( \nabla \phi = (\phi_2 - \phi_1)/h \). We now use the boundary conditions (11) and (12),

\[
(\alpha + \beta)v = \alpha \beta \left( mn(\phi_2 - \mu^L) + S(T_2 - T^L) + \frac{mn}{\rho} \lambda_{zz1} + \left( 1 - \frac{mn}{\rho} \right) S(T^W - T_1) \right)
= \alpha \beta \left\{ mn(\phi_2 - \phi_1) + S(T_2 - T_1) + S(T^W - T^L) + mn \left( \phi_1 - \mu^L + \frac{1}{\rho} \left( \lambda_{zz1} - S(T^W - T_1) \right) \right) \right\}
= \alpha \beta \left\{ -\rho_K h \frac{v}{\tau_U} + S(T^W - T^L) + mn \left( \frac{1}{\rho} \left( \lambda_{zz1} - S(T^W - T_1) \right) + \phi_1 - \mu^L \right) \right\}.
\]

In other words,

\[
v \left( \frac{1}{\alpha} + \frac{1}{\beta} + \frac{\rho_K h}{\tau_U} \right) = S(T^W - T^L) + mn \left( \frac{1}{\rho} \left( \lambda_{zz1} - S(T^W - T_1) \right) + \phi_1 - \mu^L \right),
\]

where (using Eqs. (10) and (14))

\[
\lambda_{zz1} = \Lambda_{zz1} - T_1 S_1 - E_1 + E_1 - \phi_1 \rho_1 = p^L - T_1 S_1 + E_1 - \phi_1 \rho_1.
\]

In equilibrium, \( \lambda_{zz1} = 0 \), \( \phi_1 = \mu^L \), and \( T^W = T^L = T_1 \). If the liquid temperature and pressure change by \( \Delta T \) and \( \Delta p \), we can write an equation for the growth rate \( v_g \),

\[
-v_g \frac{\rho}{mn} \left( \frac{1}{\alpha} + \frac{1}{\beta} + \frac{\rho_K h}{\tau_U} \right) = -S \Delta T
+ mn \left( \frac{1}{\rho} (\Delta p - S \Delta T_1 - T \Delta S_1 + \Delta E_1 - \rho \Delta \phi_1 - \phi \Delta \rho_1 + S \Delta T_1) + \Delta \phi_1 + \frac{S^L \Delta T - \Delta \rho}{\rho^L} \right)
= -S \Delta T + mn \left( \frac{\Delta p}{\rho} + \frac{S^L \Delta T - \Delta \rho}{\rho^L} \right) = - \left( S - S^L \frac{mn}{\rho^L} \right) \Delta T + mn \left( \frac{1}{\rho} - \frac{1}{\rho^L} \right) \Delta \rho,
\]

where we used Eq. (3), the thermodynamic equality \( d\mu = (dp - SdT)/\rho \) for the liquid, and the obvious relation \( v_g = -mn \rho/\rho \).

We now consider this equation with the second term in the right-hand side equal to zero. This is a usual scenario for heat conductivity measurements. The heat flux \( Q = vTS \) can then be expressed as

\[
Q = -\frac{\Delta T}{R_{K1} + R_{K2} + h/\kappa},
\]

where \( R_{K1} \) and \( R_{K2} \) are the Kapitza thermal resistances on the solid–wall and solid–liquid boundaries and \( \kappa \) is the heat conductivity of the crystal. Taking the inequalities \( R_{K2} \ll R_{K1}, \) \( mn \ll \rho \), and \( \rho - \rho^L \ll \rho \) into account, we immediately obtain

\[
R_{K1} = \frac{1}{\beta T S^2}, \quad \kappa = \frac{\tau_U T S^2}{\rho K}.
\]

As a result, the growth rate is given by

\[
v_g = \frac{mn}{\rho(TS^2 R_K + TS^2 h/\kappa)} \left( S \Delta T + mn \frac{\rho - \rho^L}{\rho^2} \Delta p \right).
\]

Strictly speaking, the last equality implies that thermodynamic properties of the crystal mainly depend on phonons, while the contribution of vacancies to the effect under consideration is limited to the mass transfer.
The growth rate here depends on the overpressure as well as on the temperature difference between the liquid and the wall.

In the real experiment [2], the temperature is lower than 100 mK. In this region, the phonon free path is much longer than the experimental cell size and the impact of phonons on the vacancy behavior is proportional to a high power of the small ratio $T/\Theta_D$. Consequently, as $\Theta_D \to \infty$, we can consider the vacancy gas as an independent component and neglect the influence of phonons on it. The crystal growth is accounted for by the presence of vacancies; hence, to estimate the growth rate in the experimental situation, we can simply substitute the vacancy-only quantities for all variables in Eq. (22). Since it seems that there were essentially no temperature gradients in the experiment, we consider the isothermal case $\Delta T = 0$.

The kinetic coefficients $\alpha$ and $\beta$ are determined by the vacancy annihilation probabilities in vacancy–surface collisions. The vacancy gas velocity $v$ at the interface should be expressed in terms of the accommodation coefficient $W$ (which is the ratio of the number of annihilated vacancies to the total number of incident vacancies) as

$$v \sim \frac{\Delta f}{f} V_T W,$$

where $\Delta f \sim fm\Delta\mu/T$ is the difference between the incident and reflected distribution functions and $V_T \sim \sqrt{T/m^*}$ is the thermal velocity. Here, $m^*$ is the effective mass near the bottom of the vacancy energy band. This mass can be estimated from the energy band width $\Delta$ as $m^* \sim \hbar^2/(a^2\Delta)$.

The accommodation coefficient $W$, like any other inelastic process probability in quasiparticle–surface interactions [11], is approximately the squared ratio of the lattice period to de Broglie wavelength,

$$W \sim \left(\frac{a}{\lambda}\right)^2 \sim \frac{T}{\Delta}.$$

We can now compare Eqs. (23), (19), and (20). For the coefficients, this yields,

$$\alpha \sim \beta \sim \frac{a}{n\hbar} \sqrt{\frac{T}{\Delta}}.$$

An estimate of the relaxation time $\tau_N$ characterizing the normal (non-Umklapp) vacancy collisions can be obtained from

$$\tau_N \sim \frac{1}{n\sigma V_T},$$

where $\sigma \sim a^2$ is the vacancy–vacancy scattering cross-section. The Umklapp relaxation time is exponentially longer $\tau_U \sim \tau_N \exp(\Delta_U/T)$, where $\Delta_U < \Delta$ is a certain energy specific to the vacancy Umklapp processes.

Using the obvious relation $\rho_K = m^* n$, we proceed to the growth rate. From Eq. (22), it follows that

$$v_g \sim \frac{m^2 n^2 (\rho - \rho^L)}{(1/\alpha + 1/\beta + m^* n/\tau_U)\rho^3} \Delta p \sim \frac{m^2 n^2 (\rho - \rho^L)}{\left(\sqrt{\Delta/Tn\hbar/a + \hbar m^* n^2 a^2 V_T \exp(-\Delta_U/T)}\right)\rho^3} \Delta p$$

$$\sim \frac{a^4 (\rho - \rho^L)}{\hbar \rho} \left(\sqrt{\frac{\Delta}{T}} e^{\epsilon_0/T} + \frac{\hbar}{a} \sqrt{\frac{T}{\Delta}} e^{-\Delta_U/T}\right)^{-1} \Delta p.$$

Here, as an estimate, we set $\rho_0^3 \sim m$ and $na^3 \sim \exp(-\epsilon_0/T)$, where $\epsilon_0$ is the bottom of the vacancy energy band. For the facet mobility $\mu_f^* = v_g/\Delta p$ introduced in [3], we have

$$\mu_f^* \sim \frac{a^4 (\rho - \rho^L)}{\hbar \rho} \left(\sqrt{\frac{\Delta}{T}} e^{\epsilon_0/T} + \frac{\hbar}{a} \sqrt{\frac{T}{\Delta}} e^{-\Delta_U/T}\right)^{-1}. \quad (24)$$

6 Conclusion

Formula (24) provides a reasonable correspondence between the theory proposed here and the experiment [3]. It suggests three main predictions to be verified in further experiments.
• The facet mobility has a maximum at some finite temperature. Should the temperature decrease below the point of the maximum, the growth rate will also decrease. Otherwise, if the mobility does not tend to zero as the temperature tends to zero, this should be considered as an indication of the presence of zero-point vacancies (see [12]).

• The observed growth rate depends on the height of the sample.

• The crystal grows at the boundary between the solid and the wall. This fact can potentially be observed experimentally using some small foreign object frozen into the crystal in its upper part.

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