CRYSTAL SHAPES VIEWED AS MECHANICAL EQUILIBRIUM OF STEPS

M. UWABA* and P. NOZIÈRES

Institut Laue-Langevin, 156X, 38042 Grenoble Cedex, France

A crystal surface below the roughening temperature $T_R$ tends to develop steps, whose thickness $\xi$ diverges at $T_R$. For a low angle vicinal surface ($\xi n < 1, n$: step density), the crystal shape is viewed as “mechanical” equilibrium of these steps. We study forces acting on a step and their relation to the crystal shape. Such an approach is extended to describe steady growth shapes under the assumption that bulk processes such as diffusion can be neglected, as is the case for $^3$He. We study, particularly, the shape and melting rate near the stability threshold of a facet and find different melting laws depending on the step interaction.

1. Introduction

The shape of a crystal in melting equilibrium with its liquid is controlled by anisotropies of the interfacial energy (actually free energy) $\gamma$. Let $\delta p_L$ be the pressure in the liquid, measured from the nominal equilibrium pressure $\rho_L^*$ for a flat interface. Melting equilibrium requires that

$$\delta p_L = \frac{\rho_L}{\rho_S - \rho_L} \left[ \gamma \delta_{\mu\nu} + \frac{\partial^2 \gamma}{\partial \theta_{\mu} \partial \theta_{\nu}} \right] C_{\mu\nu},$$

(1)

where $C_{\mu\nu}$ is the local curvature tensor.\(^1\) In the simple case of a cylindrical interface with a single curvature, (1) reduces to the familiar result

$$\delta p_L = \frac{\rho_L}{\rho_S - \rho_L} \frac{\gamma + \gamma''}{R},$$

(1')

\(^1\)Present address: Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Sendai 980, Japan.

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where \( R \) is the radius of curvature.* If the sample is small, \( \delta p_L \) may be considered as constant, and Eq. (1) fixes the geometry through the local curvature. When the size exceeds the capillary length, one must take care of the hydrostatic pressure shift and the interface tends to flatten.

For a sample completely surrounded by liquid, Eq. (1) has an elegant geometrical solution, the famous Wulff construction.\(^2\) An equivalent thermodynamic language was recently devised by Andreev, using an appropriate Legendre transformation of the surface energy.\(^3\) In more practical situations, the interface touches walls, which provide boundary conditions through fixed contact angles. The search of an equilibrium shape then becomes quite complicated, although difficulties are purely mathematical.

This thermodynamic formulation is self-sufficient, but it is often untractable and not very transparent. The purpose of this paper is to show that in many cases crystal shape may be interpreted as an equilibrium of steps. In a way, no new result will emerge—but the language will be much simpler, and the physics will be more obvious.

The concept of steps only makes sense if they are well-separated, i.e. if their distance \( d \) exceeds their width \( \xi \) (the coherence length of the corresponding roughening transition at \( T_{R_0} \)). That implies first \( T<T_{R_0} \) (otherwise \( \xi \) is infinite). Moreover, the angle \( \theta \) between the interface and the crystal planes must be small enough. Since \( \theta \sim a/d \) (where \( a \) is the lattice spacing), well-defined steps only exist for vicinal surfaces such that \( \theta\sim a/\xi \). For larger angles, thermal fluctuations blur the step structure: the rough interface should then be viewed as a random distribution of fluctuating terraces. The present discussion is only concerned with vicinal surfaces. Close to \( T_R \), this is a drastic restriction, since \( \xi \) diverges rapidly. At low temperature, however, \( \xi \) is small and our picture makes sense in a broader angular range.

When talking about a step, we refer to a given crystal plane—say the (001) crystal plane in a cubic crystal. Facets may, of course, also occur for other orientations: when referred to the original (001) plane, these higher facets correspond to a commensurate arrangement of the step density \( n \) in the periodic potential of that plane while a single step was a consequence of the periodicity perpendicular to the (001) plane, higher order facets result from the periodicity parallel to that plane. At low temperature one cannot ignore the latter. If, however, \( T \) is larger than the roughening temperature of that higher index face in-plane periodicity becomes irrelevant and one may ignore it. The crystal appears as a stack of plates, with no “in-plane structure”. The

\(^*\)The occurrence of \( \tilde{\gamma} = \gamma + \gamma' \) in (1') may be interpreted as resulting from effective stresses acting on a surface element, as shown on Fig. 1 (as regards melting, the solid behaves as an anisotropic fluid, and we may ignore the complicated elastic surface stresses\(^4\)). Besides the usual stretching force \( \gamma \), a torque \( \gamma' \) tends to rotate the surface towards orientation of lower energy. For a bent element (radius \( R \)), it is easily verified that the total tangential force is zero, while the normal component is \((\gamma + \gamma')/R \).
(001) steps will move freely, without being hindered by any periodic potential. For small $\theta$, $T_R$ of high Miller index planes is very small, and the approximation is very good. If $\theta$ approaches $45^\circ$, however, one must start worrying.

To summarize this discussion, we consider only steps with respect to a single crystal plane, which move continuously in that plane. Any higher commensurate order is neglected, an approximation which is good for small $\theta$. As regards temperature, our model is sandwiched between two conflicting limits: $T$ must be smaller than the $T_{R0}$ (for steps to make sense), but larger than higher $T_R$'s (for the in-plane periodicity to be negligible). Within these limits, the “stack of smooth plates” model makes sense.

2. **Equilibrium Shape of a Cylindrical Interface**

We first consider the simplest geometry: a cylindrical interface with a single curvature, made up of parallel straight steps. Consider a unit distance $dx$ along the crystal planes; the step density $n(x)$ is related to the orientation

$$\tan \theta = -na,$$

(where $a$ is the lattice spacing; see Fig. 2), while the free energy density $E(n)$ yields the surface energy:

$$\gamma(\theta) = \cos \theta \ E(n) = \cos \theta \ E \left( -\frac{\tan \theta}{a} \right).$$
For small $n$, we may expand $E(n)$:

$$E = \gamma_0 + \beta n + \phi n^p + .....$$

(2)

$\gamma_0$ is the original facet energy. $\beta$ is the free energy of a single step, the next terms correspond to step interactions. Within a virial-like expansion, it would appear natural to set $p=2$. In fact, steps are macroscopic entities, a distance $d= n^{-1}$ apart: their interaction energy is controlled by the average configuration. It is known that the main interaction goes as $1/d^2$, arising partly from the elastic deformation of the substrate, partly from the confinement of statistical fluctuations. As a result, the main interaction term is $\phi n^3$—a feature which will have important consequences.

If the liquid overpressure $\delta p_L$ is positive, the solid tends to grow. A single step (corresponding to $\theta<0$) is thus subject to an external force (per unit length)

$$F = a\rho_S \left( \mu_L - \varepsilon_S - \frac{1}{\rho_S} \rho_L \right) = \delta p_L a \frac{\rho_S - \rho_L}{\rho_L}$$

(3)

($\rho_L, \rho_S$ are mass densities, $\mu_L, \varepsilon_S$ liquid chemical potential and solid energy density per unit mass). Unless there are no steps at all (flat facet), this force $F$ must be balanced by the repulsion of other steps, in order to achieve equilibrium. Let us define a step chemical potential

$$\zeta(n) = \frac{dE}{dn} = -ad[\gamma \sin \theta + \gamma' \cos \theta].$$

(4)

The interaction force is
\[ F' = -\frac{\partial \zeta}{\partial x} = -E''(n) \frac{\partial n}{\partial x}. \]

Equilibrium requires \( F' + F = 0 \). It is easily seen that

\[
\gamma + \gamma'' = \frac{E''}{a^2 \cos^3 \theta}, \quad \frac{1}{R} = -\frac{d\theta}{ds} = a \cos^3 \theta \frac{dn}{dx}.
\]

The condition \( F' + F = 0 \) is thus identical to the usual criterion (1'): the equilibrium shape results from mechanical equilibrium of steps. The correspondence is complete: for instance, the local stability condition, \( \gamma + \gamma'' > 0 \), simply means that the step compressibility is positive: \( E'' > 0 \).

2.1 Contact with a wall

If the wall is parallel to the crystal axis, it simply acts as a source of steps, thereby fixing the step chemical potential:

\[
\zeta_w = a(\gamma_S - \gamma_L) \tag{5}
\]

(where \( \gamma_S \) and \( \gamma_L \) are the interfacial energies of the two phases with the wall). If the crystal makes an angle \( \alpha \) with the wall (Fig. 3), a virtual displacement of the contact point A also modifies the area available to preexisting steps. The boundary condition will then involve a combination of the step “chemical potential” \( \zeta \) and the step pressure.

![Diagram](Fig. 3. Geometry of the contact with a wall.)
\[ \Pi = n\zeta - E = \gamma'\sin\theta - \gamma\cos\theta. \]  \hfill (6)

Requiring that the energy be stationary, it is easily verified that the boundary condition at A reads

\[ \zeta \cos\alpha + \Pi a \sin\alpha = a(\gamma_s - \gamma_l). \]  \hfill (7)

(7) fixes the contact angle, which in the present language reflects the "nucleation-compression" equilibrium of steps at the wall: We assume the contact angle is finite in what follows.

Note that \( \zeta \) and \( \Pi \) given by (4) and (6) have a simple physical interpretation in terms of effective surface stresses. According to Fig. 1, \( -\Pi \) is nothing but the component of stress parallel to crystal planes (the one that involves compression of preexisting steps). Similarly \( -\zeta/a \) is the component perpendicular to crystal planes (whose work implies step creation). In that picture, \(^6\) (7) is just the balance of forces at A.

2.2 Faceting

Let \( \zeta_w \), be the value of \( \zeta \) at the wall, fixed by the boundary condition (7). A distance \( x = -|x| \) from the wall along the crystal planes, \( \zeta \) decreases linearly as

\[ \zeta(x) = \zeta_w - F|x|. \]

The step density goes down to a threshold where a facet is formed (step "vacuum"). Beyond that threshold, the problem of force balance is irrelevant, since there is no step. Two cases are possible:

(i) Usually, \( \zeta(n) \) is monotonous (Fig. 4(a)). \( \zeta \) decreases to its lower bound \( \beta \), corresponding to \( n=0 \). The round part thus matches tangentially to a flat facet, the width of the round part being

\[ |x_o| = \frac{\zeta_w - \beta}{F}. \]  \hfill (8)

Near the edge of the facet, \( \zeta - \beta = 3\phi n^2 \). Hence the profile is such that

\[ \theta \approx -na \approx -\sqrt{\frac{F\alpha(x - x_o)}{3\phi}}. \]

The resulting \( z \sim (x-x_o)^{3/2} \) shape is a direct consequence of the \( 1/d^2 \) interaction between steps (observable only if \( |\theta| \) is smaller than \( a/\zeta \), a stringent condition near \( T_{R\theta} \)).

(ii) It may also happen that \( \zeta(n) \) has a minimum (implying some sort of long range attraction between steps). Then a "first order" contact develops
between a step "liquid", with finite density $n_0$, and a flat fact $n=0$. $n_0$ is fixed by the requirement that $\Pi$ be the same in both phases (the tangent in Fig. 4(b)). As a result the contact of round and faceted regions is angular instead of tangential—a situation often encountered in practice.* Note that $\zeta<\beta$ at the edge: the width $|x_0|$ of the round part is enlarged as compared to (8).

2.3 Size of the facet

We consider the simplest case: two parallel walls a distance $2L$ apart, parallel to the crystal axis (we are neglecting gravity). The width $2l$ of the facet is then what is left by the round parts (Fig. 5):

*Angular points may also appear inside round parts, as soon as $E(n)$ possesses double tangents (this means $\zeta(n_1)=\zeta(n_2)$, $\Pi(n_1)=\Pi(n_2)$). The situation is similar to a liquid-gas separation: orientations corresponding to a negative step compressibility, $E^*<0$, are forbidden—hence a discontinuous profile.
\[ l = L - |x_0| = L - \frac{\zeta_w - \beta}{F} \]  \hspace{1cm} (9)

(we assume tangential matching at facet edge for simplicity). If \( F \) is too small, i.e. if

\[ \delta p_L < \delta p_L^* = \frac{\rho_L}{\rho_S - \rho_L} \frac{\zeta_w - \beta}{aL}, \]  \hspace{1cm} (10)

the facet shrinks to nothing, and there exists no equilibrium configurations: the crystal steadily melts, steps converging from both sides towards the center. If \( \delta p_L > \delta p_L^* \), a stable state is on the contrary possible, but it only corresponds to metastable equilibrium on each side: the nucleation of a step-antistep pair (i.e. of a terrace above the facet) is ignored. In real equilibrium, the energy must be stationary under the latter process as well—hence a further condition

\[ 2\beta - 2LF = 0, \]  \hspace{1cm} (11)

which is equivalent to stating that the extrapolated \( \zeta \) vanishes at the center of the cell. Combining (9) and (11), we see that strict equilibrium is only possible for a specific \( \delta p_L \):

\[ \delta p_L^{eq} = \frac{\rho_L}{\rho_S - \rho_L} \frac{\zeta_w}{aL}. \]  \hspace{1cm} (12)
This is Jurin’s law of capillary rise in a different garb.

3. Interfaces with an Axis of Revolution

We consider a circular cylinder vessel (radius $L$), into which a crystal grows with its axis parallel to that of the vessel. If we neglect anisotropies in the crystal planes, the interface is axially symmetric, and the steps are concentric circles, with a density $n(r)$. Each unit length of step is now subject to three radial forces:

- The external overpressure force $F$ (outward)
- The interaction with its neighbours $-\frac{\partial \zeta}{\partial r}$
- A tension force due to step curvature, equal to $-\frac{\zeta}{r}$.

The equilibrium condition thus reads as

$$\frac{d\zeta}{dr} + \frac{\zeta}{r} = F. \quad (13)$$

Integration of (13) yields at once

$$\zeta = \frac{Fr}{2} + \frac{2\zeta_w L - FL^2}{2r},$$

from which the profile $n(r)$ is inferred. The edge $R$ of the face corresponds to $\zeta(R)=\beta$, as shown on Fig. 6 for various values of $F$. The solution disappears

![Diagram](image.png)

**Fig. 6.** The profile $\zeta(r)$ for an axially symmetric interface for various values of $F$. The curve 3 corresponds to collapse threshold ($\text{Min}\zeta=\beta$). The curve 2 corresponds to thermodynamic equilibrium.
below a threshold $F_c$ for which $\text{Min } \zeta = \beta$. At threshold,

$$F_c L = \zeta_w + \sqrt{\zeta_w^2 - \beta^2}, \quad R_c = \frac{\beta}{F_c}.$$ (14)

Below $F_c$, the overpressure $F$ can no longer counter the line tension $\beta/R$ of the last steps near the edge: the facet collapses, steps pouring in continuously towards the center—the crystal steadily melts. Observation of this melting threshold is probably the neatest way to reach the step energy $\beta$ experimentally (equilibrium sizes are usually plagued by metastability and hysteresis).

An additional terrace with radius $r$ costs an energy

$$\Delta E = 2\pi r \beta - \pi r^2 F.$$ (15)

Collapse is reached when the facet radius $R$ corresponds to the top of that nucleation barrier (edge steps spontaneously shrink). In contrast, thermal equilibrium is achieved if $\Delta E = 0$ for $r = R$ (nucleation of a terrace is balanced). At a given $F$, the equilibrium facet radius $R_{eq}$ is thus twice the collapse radius $R_c$. The corresponding profile $\zeta(r)$ is linear (curve “2” in Fig. 6). The final behaviour of $R$ as a function of $F$ is sketched on Fig. 7.

The step picture thus works equally well for an axially symmetric interface. The only new feature is the tension force due to step bending, leading to the important phenomenon of collapse at finite $F_c$ and $R_c$. Generalization to a completely anisotropic situation is possible (anisotropy in $\beta$ and in the step distribution $n(r)$). The formulation is however less simple and thus less appealing: it is sketched in Appendix A.

![Graph showing facet radius as a function of the overpressure force $F$](image_url)

**Fig. 7.** Facet radius as a function of the overpressure force $F$
4. Steady Growth Shapes

In most materials, growth dynamics is controlled by bulk diffusion, either of the latent heat or of chemical species in a mixture. We focus here on the opposite limit, while growth is monitored by interface dissipation only. We are interested in a steady state in which the solid grows at a constant velocity $V$ along the $z$-axis. Let $\Phi$ be the net force acting on a step (overpressure, interactions, line tension). If $\Phi \neq 0$, the step moves at a velocity $u = \eta \Phi$, where $\eta$ is its mobility—hence a velocity $v_z$ perpendicular to the crystal planes $V = n a u$; the interface goes up by $a$ whenever a step goes by. The growth rate is controlled by the mobility of individual steps for small $\theta$, and vanishes if $\theta = 0$. (When $\theta$ increases, dissipation becomes more collective, and the concept of a step mobility becomes doubtful.)

A steady shape growing along the crystal axis corresponds to $V = \text{const}$, i.e. to

$$\Phi(n) = \frac{V}{\eta a n}. \quad (16)$$

This is a first order differential equation for the step density $n(x)$—hence for the profile.

As an example, let us consider the situation just beyond the collapse threshold of a circular facet. Equation (16) then reads

$$\frac{d\zeta}{dr} + \frac{\zeta}{r} + \frac{V}{\eta a n} = F \quad (17)$$

($\zeta$ being a given function of $n$). Close to the threshold $F_c$, it is clear that all the physics will be localized near the facet edge, $r = R_c$, where steps “hesitate” on what to do. When $r \gg R_c$, the round part is nearly in equilibrium and $V$ can be neglected in (17):

$$\zeta \approx \frac{F_c r}{2} + \frac{\beta^2}{2 F_c r} + \frac{(F_c - F)}{2r} (L^2 - R_c^2) + \ldots$$

When $r \ll R_c$, instead, steps are very few and their interaction may be ignored—i.e. $\zeta = \beta$:

$$n = -\frac{V}{\eta a F} \frac{r}{R_c - r}.$$

The only problem is to match these two limiting forms near $r = R_c$. This is done
explicitly in Appendix B, using a simple expansion in powers of \((F_c - F)\). As expected, growth begins at \(F_c\). Near \(F_c\), the flat facet is slightly "domed" (parabolic) by steps which keep pouring in. The growth characteristic \(V(F)\) depends critically on the step interaction near the edge (it is that interaction which drives the steps through into the facet). With a \(1/d^2\) interaction—i.e., \(\zeta(n) = \beta + 3\phi n^2 + ...\) \((p=3)\), the growth law is linear near threshold:

\[ V \sim (F_c - F). \]

If instead we had chosen \(\zeta(n) = \beta + 2\phi n + ...\) \((p=2)\), virial-type expansion, we would have obtained

\[ V \sim (F_c - F)^{3/2}. \]

The behaviour of \(V(F)\) near collapse thus yields direct information on the nature of step repulsion on vicinal surfaces.

A similar analysis may be carried out for the one-dimensional geometry of a cylindrical interface, when the "stripe" facet width reduces to zero: steps of opposite sign meet and annihilate at the center. The curvature term disappears in (17), and the differential equation is trivial. The only difficulty lies in the boundary condition at the center. If we assume an instantaneous recombination of opposite steps, we are let to write \(n(x=0)=0\). The resulting growth law is

\[ V \sim \frac{F_c - F}{\log(F_c - F)} \quad \text{for} \ p = 2, \quad V \sim (F_c - F) \quad \text{for} \ p = 3. \]

Here again, the nature of step interactions is reflected in macroscopic quantities. In practice, such a boundary condition is too crude: the annihilation takes a finite time \(\tau\), controlled by the short range elastic attraction of opposite steps—as a result, \(n(0)\neq 0\)—a correction which is negligible near threshold (one may show that \(n(0) \sim V^{1/4}\)).

The conclusion of this brief discussion is that growth laws near collapse thresholds are sensitive to details of the surface energy, such as step interaction terms. The reason is that the whole process is controlled by those tiny regions where equilibrium is marginal.

Appendix A: Forces Acting on a Step

Let \((x, y)\) be the reference crystal plane: we consider an arbitrary interface which on a gross scale has position \(z(x, y)\). The steps are then the constant height curves on which \(z\) is a multiple of \(a\). It is convenient to define a step density vector
\[ n = \frac{1}{a} \text{grad } z. \]

\( n \) is perpendicular to the steps, its modulus \( n=1/d \) is the step density (Fig. 8). The surface geometry is fixed by the distribution \( n(x, y) \) and \( \phi(x, y) \) (where \( \phi \) is the azimuthal angle of \( n \)). Let \( \hat{n} \) and \( \hat{t} \) be the unit vectors normal and tangential to the steps. The geometry embodies three basic features:

(i) \( G=(\hat{n} \cdot \text{grad})n \) measures the gradient in step spacing (already present in one dimension)

(ii) \( D=(\hat{n} \cdot \text{grad})\phi \) measures the divergence of the steps (because curl \( n=0 \), \( D \) is also equal to \( 1/n(\hat{t} \cdot \text{grad})n \))

(iii) \( 1/R=(\hat{t} \cdot \text{grad})\phi \) measures the curvature of the steps.

We want to calculate the forces acting on a step in terms of \( G, D, R \).

Let \( E=n\phi(n, \phi) \) be the step energy per unit area in the crystal plane. Equilibrium is achieved by minimizing the total energy

\[ \iint dx dy \left( E - \frac{F}{a} \right). \]

Let us introduce a chemical potential vector

\[ \zeta = \frac{dE}{dn} = \zeta \hat{n} + \epsilon \phi \hat{t} \]

with

\[ \text{Fig. 8. Unit vectors related to the step direction.} \]
\[ \zeta = \varepsilon + n \frac{\partial \varepsilon}{\partial n}, \quad \varepsilon_\phi = \frac{\partial \varepsilon}{\partial \phi}. \]

The resulting Euler equation is simply \( \text{div} \zeta = -F \). (Note that it is a scalar equation, expressing pressure equilibrium). Making use of the identities

\[ \text{div} \hat{n} = (\hat{i} \cdot \text{grad}) \phi = \frac{1}{R}, \quad \text{div} \hat{i} = -(\hat{n} \cdot \text{grad}) \phi = -D, \]

the equilibrium equation becomes

\[ F + \frac{\partial \zeta}{\partial n} G + \left( \zeta + \frac{\partial^2 \varepsilon}{\partial \phi^2} \right) \frac{1}{R} + 2n \frac{\partial^2 \varepsilon}{\partial n \partial \phi} D = 0. \quad (A.1) \]

We recognize the various forces acting on a step element, due to the density gradient \( G \) or to the curvature \( R \). The new feature is the last term, proportional to the divergence \( D \), which originates in the anisotropy of the step interaction (\( \partial \varepsilon / \partial n \) would be zero if the step were independent).

Although (A.1) is self-contained, it is instructive to interpret it in terms of detailed forces. As shown on Fig. 9 a given step element is subject to three sets of forces

(i) A stretching tension \( \zeta \) parallel to the step
(ii) A rotation torque \( \varepsilon_\phi \) (note that \( \varepsilon_\phi \) enters rather than \( \partial \zeta / \partial \phi \))
(iii) A “bulk” force per unit length of step

\[ \Phi = -\frac{\partial \zeta}{\partial n} \text{grad} \ n - \frac{\partial^2 \varepsilon}{\partial n \partial \phi} \ n \text{grad} \ \phi \]

\[ = -[\text{grad} \zeta - \varepsilon_\phi \text{grad} \phi]. \]

**Fig. 9.** Forces acting on a step.
(i) and (ii) are the analogue for a step of the stresses found for a surface element in Fig. 1. The new feature is the bulk force $\Phi$, which is basically the "interaction" part of $-\text{grad}\zeta$. Let $x$ be the direction of the step (parallel to $\hat{n}$). The net tangential force acting on the step element is

$$\int d\mathbf{x} \left( \frac{\partial \zeta}{\partial x} - \varepsilon_\phi \frac{\partial \phi}{\partial x} + \Phi_x \right) = 0$$

(as it should). The net normal component is instead

$$\int d\mathbf{x} \left( \zeta \frac{\partial \phi}{\partial x} + \frac{\partial \varepsilon_\phi}{\partial x} + \Phi_x \right) = -\text{div} \zeta.$$

When balanced with the overpressure force $F$, it yields our former equilibrium condition (A.1). The physical nature of the forces acting on a step is thus clarified.

**Appendix B: Melting Velocity Near Threshold**

Let $\zeta = \beta + \lambda \eta^q + ... (\lambda = p\phi, q = p - 1; \text{see (2)})$. We discuss some properties of the solution of the nonlinear differential equation

$$\frac{d\zeta}{dr} + \frac{\zeta}{r} + \frac{V}{\eta a} \left( \frac{\lambda}{\zeta - \beta} \right)^{1/q} = F$$  \hspace{1cm} (A.2)

with the boundary conditions

$$\zeta(0) = \beta, \quad \zeta(L) = \zeta_w$$  \hspace{1cm} (A.3)

in the limit that $F \rightarrow F_c$.

By the scale transformation

$$x = \frac{F}{\beta} r, \quad y = \frac{\zeta}{\beta},$$

Equation (A.2) becomes

$$\frac{dy}{dx} + \frac{y}{x} - \frac{\alpha}{(y - 1)^{1/q}} = 1.$$  \hspace{1cm} (A.2')

Here $\alpha$ is the scaled melting velocity.
\[ \alpha = \frac{V}{\eta a F} \left( \frac{\lambda}{\beta} \right)^{1/q}, \]

which is a small parameter in the present problem. The boundary conditions (A.3) become

\[ y(0) = 1, \quad y \left( \frac{FL}{\beta} \right) = \frac{\zeta_w}{\beta}. \]

The solution at threshold is written as

\[ y_c(x) = \frac{1}{2} \left( x + \frac{1}{x} \right) \]

for \( x \geq 1 \) \((x_c \equiv F_c R_c / \beta = 1)\). Beyond threshold the two limiting forms of \( \zeta(r) \) are

\[ y(x) = 1 + (\alpha x)^q \]

for \( x \rightarrow 0 \), and

\[ y(x) = y_c(x) + \frac{F - F_c}{F_c} \frac{x^2 - (L/R_c)^2}{2x} + O(\alpha) \quad (A.4) \]

for \( x \rightarrow L/R_c \). In order to find the matching condition near \( x = 1 \) and \( y = 1 \) we put

\[ x = 1 + \alpha^{q/(q+2)} X, \]
\[ y = 1 + \alpha^{2q/(q+2)} Y. \]

In leading order Eq. (A.2') becomes

\[ \left( \frac{dY}{dX} - X - \frac{1}{Y^{1/q}} \right) = 0. \quad (A.5) \]

For \( X \rightarrow -\infty \) \((Y \rightarrow \infty)\) all solutions of (A.5) have the form

\[ Y = \frac{1}{2} (X^2 + A), \quad (A.6) \]

which is consistent with the quadratic behavior of (A.4) near \( x = 1 \). Among them only one solution satisfies the correct limit

\[ X \rightarrow -\infty, \quad Y \rightarrow 0. \]
The asymptotic form of the solution is

$$Y = \left(-\frac{1}{x}\right)^q.$$

In Fig. 10 we show the solution for $q=1$, of which the constant $A$ of (A.6) is about 5.4.

Comparing (A.4) and (A.6), we see that the constant $A$ is basically $(F - F_c)$ appropriately scaled. Detailed identification yields the following growth law, valid for small $\alpha$ (near threshold) and $q=1$ ($p=2$)

$$V = \eta n_w a F_c \frac{\beta}{\zeta_w} - \beta \left[ \frac{1 - (L/R_c)^2}{A} \right]^{3/2} \left( \frac{F_c - F}{F_c} \right)^{3/2},$$

where $n_w$ is the step density at the wall. For $q=2$ ($p=3$) the numerical coefficient cannot be determined by this method and we obtain

$$V \approx \eta n_w a (F_c - F).$$

Fig. 10. Solution of $dY/dX = X + (1/Y)$ and its asymptotic forms.
REFERENCES


DISCUSSION

Müller-Krumbhaar

Does your analysis indicate, that the facet of a crystal (in a container) may disappear, before the theoretical roughening point is reached?

A: Yes. Near the disappearance of facet ($F \approx F_c$), however, the curvature of the central part ($r \approx R_c$) is so small that it is very difficult to distinguish it from a facet. Practically, a melting “quasi-facet” may be seen (see Fig. 10).

Kirkpatrick

Do these phenomena take place in the crystal-stable portion of the ordinary phase diagram?

A: Yes.

Van der Eerden

Can the method of treating step interaction as a mechanical problem be used to calculate the influence of interaction on the spiral growth law? If yes, have an expression for the correction to the parabolic law: “rate of growth” $\sim (\Delta \mu / k T)^2$.

A: We have studied the growth of facet based on a similar picture and found a different growth law in the region where $F$ is very close to the Frank-Read threshold (although the step interactions are not relevant).

Ming

What is the physical meaning of mechanical force in atomic scale? I mean
that if the steps are monomolecular step, what is the meaning of mechanical force.

A: The word "mechanical force" may be slightly misleading. One of the forces I mentioned is elastic interaction, which is purely mechanical, but the other force is due to the fluctuation of steps and statistical nature.

Chernov

Do you know any attractive interaction of steps?

A: No. But, I don't see any reason to exclude that possibility.

Bennema

Can these ideas be applied to sphere experiments, where you make from a single crystal a sphere and then let this crystal grow for a short time. So you study the relative strength of the faces.

A: In principle it is possible to apply the same idea. In practice it is convenient to choose a geometry that has translational symmetry (in the z-direction) because we can have a steady state.