The roughening transition of crystal surfaces. I. static and dynamic renormalization theory, crystal shape and facet growth

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Résumé. — Le traitement de la transition rugueuse par une méthode de renormalisation est repris à la base, tant dans le cas statique que dans le cas dynamique. Les résultats antérieurs fondés sur une approximation asymptotique sont corrigés, en particulier en ce qui concerne la mobilité. Pour un interface incliné, ou en présence d'une force appliquée F, il apparaît une nouvelle échelle de longueur, qui doit être comparée à la longueur de corrélation ξ. De ce fait, la transition rugueuse est *étalée*, la transition progressive se situant en dessous de T_R. Nous approchons cette transition par les deux bouts, par une technique de « renormalisation bloquée » du côté rugueux, dans un schéma de « marches discrètes » du côté facetté. A ce dernier stade, la discussion est surtout qualitative. La comparaison avec l'expérience sera faite ailleurs.

Abstract. — The renormalization approach to the roughening transition is reconsidered, both in a static and in a dynamic picture. Earlier results based on an asymptotic approximation are corrected, especially as regards the interface mobility. For a tilted interface, or in the presence of an applied force F, a new length scale appears, which must be compared to the correlation length ξ. As a result, the roughening transition is *blurred*, the crossover occurring below T_R. This crossover is approached from both ends, *via* a « stopped renormalization » technique on the rough side, within a « discrete step » picture in the faceted state. At this last stage, the discussion is mostly qualitative. Comparison with experiment is done elsewhere.

The existence of a roughening transition of planar crystal surfaces was predicted long ago by Burton, Cabrera and Frank [1]. It is now well established that this transition is of the type described by Kosterlitz and Thouless [2, 7, 9] in a different context. Standard theories are based on a renormalization group approach, in which the length scale is progressively enlarged [3]. Such a renormalization may be carried out either in real space, or more conveniently in momentum space [4], by elimination of short wavelength fluctuations of the surface. However, such a momentum renormalization must be carried out carefully [5], and in this respect, much of the existing literature is incorrect. Moreover, all existing calculations rely on a « logarithmic » approximation, which is only correct at the transition temperature itself. In order to interpret recent experimental results on the roughening of ^{4}He facets at the transition and away from the transition, one needs a more systematic theoretical picture.

In the present paper, we first reconsider the renormalization theory of a *static* roughening transition. We extend it to a vicinal surface with a finite tilt angle θ and, for $T < T_R$, we analyse the transition from a « rough » behaviour at large θ to a discrete step regime at small θ. We then turn to the *dynamic* behaviour of the surface, i.e. its response to an applied overpressure. That problem was considered by Chui and Weeks [6], who demonstrated a crucial result : the dynamics is « conventional », in the sense that the mobility remains finite at T_R. Their approach, however, is exact only at $T = T_R$, as usual with renormalization methods : we shall see that it may be significantly improved away from T_R. More generally, we shall discuss both the linear mobility at $T > T_R$ and the transition towards a non linear homogeneous nucleation regime at $T < T_R$.

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These results are used in order to interpret experiments in ^{4}He in the accompanying paper [10].

The main purpose of the present paper is to expound explicitly, to correct and to extend ideas which are present in the literature, in a way which allows comparison to experiment.

1. Static renormalization.

We consider a planar interface, whose height fluctuations are described by a profile $z(\mathbf{r})$. The corresponding energy is

$$E(z) = \iint d^2r[\gamma (\text{grad } z)^2/2 - V \cos (2 \pi z/a)]$$

(1)

where a is the lattice spacing normal to the surface, γ the *surface stiffness*, related to the surface *energy* $\alpha(\theta)$ according to

$$\gamma = \alpha + (d^2\alpha/d\theta^2).$$

The pinning potential V tends to fix the interface at integer values of z/a. In order to give (1) a meaning, we need a *cut off*. Following Knops *et al.* [5], we assume that equilibrium fluctuations for $V = 0$ are such that

$$\langle z_k^2 \rangle = (T/\gamma k^2) f(k/\Lambda_0).$$

(2)

The original cut off Λ_0 is $\sim a^{-1}$; the form factor $f(x)$ goes to 1 if $x \to 0$, to 0 if $x \gg 1$: its precise shape is irrelevant (sharp step function or smooth cut off). Technically, (2) is achieved by the replacement $\gamma \to \gamma/f$ in (1).

In a *renormalization transformation*, we write $z = \bar{z} + \delta z$, in such a way that in zeroth order (in V)

$$\langle \bar{z}_k^2 \rangle = (T/\gamma k^2)(1 - \psi) f$$
$$\langle \delta z_k^2 \rangle = (T/\gamma k^2) \psi f$$

($\psi(\Lambda_0)$ will eventually be made infinitesimal).

We can formally introduce the following Hamiltonian :

$$E'(\bar{z}, \delta z) = \sum_k (\gamma k^2/2 \ f)[(\bar{z}_k^2/(1 - \psi)) + (\delta z_k^2/\psi)] -$$
$$- \iint d^2r \ V \cos (2 \pi(\bar{z} + \delta z)/a)$$

(3)

in which $\bar{z}_k$ and δz_k are now *independent* statistical variables. It is easily verified that (1) and (3) are equivalent, in the sense that they yield the same partition function Z

$$Z = \int d\bar{z}_k \int d \ \delta z_k \exp(- E'/T).$$

(4)

(If we carry the summation over δz_k first *at constant z_k*, we recover the partition function of (1) within an irrelevant constant factor : (1) and (3) are physically equivalent).

The spirit of renormalization is to eliminate δz by integrating (4) over δz_k at constant $\bar{z}_k$, thereby defining an *effective energy* $\bar{E}$ for the truncated fluctuations $\bar{z}_k$

$$Z = \int d\bar{z}_k \exp[- \bar{E}(\bar{z}_k)/T].$$

The periodic potential $V = V \cos (2 \pi z/a)$ creates a mode-mode coupling, so that

$$\bar{E} = \gamma k^2 \bar{z}_k^2/(2(1 - \psi) f) - T \log \langle (\exp(V/T)) \rangle \quad (5)$$

where $\langle \ \rangle$ denotes a Gaussian average over δz_k. (5) is still exact : in order to proceed, we expand in powers of V

$$- T \text{Log} \langle \exp(V/T) \rangle \to - \langle V \rangle - (1/2 \ T) \times$$
$$\times [\langle V^2 \rangle - \langle V \rangle^2] + \cdots \quad (6)$$

The expression (6) is the basic approximation of the theory, valid for weak coupling $V \ll T$.

From now on, the algebra is standard. Since it is done elsewhere [3], we only sketch it. We introduce a correlation function

$$\delta g(\rho) = (2 \pi \gamma/T)\langle \delta z(r) \ \delta z(r + \rho) \rangle =$$
$$= \int_0^\infty (dk/k) J_0(k\rho) \ \psi f.$$

(J_0 is the zeroth order Bessel function) from which we infer

$$\langle \cos (2 \pi \ \delta z/a) \rangle = \exp[- (2 \pi^2/a^2)\langle \delta z^2 \rangle] =$$
$$= \exp[- n \ \delta g(0)].$$

The dimensionless quantity $n = \pi T/\gamma a^2$ will be crucial in what follows. The first order correction to $\bar{E}$ is simply a *renormalized periodic potential*, with a strength

$$\bar{V} = V \exp(- n \ \delta g(0))$$

reduced by the fluctuations δz. In second order, we find

$$\bar{E}^{(2)} = - \iint d^2r \ d^2r'(\bar{V}^2/4 \ T) \times$$
$$\times [\cos (2 \pi(\bar{z} + \bar{z}')/a)\{\exp(- 2 n \ \delta g(\rho)) - 1\} +$$
$$+ \cos (2 \pi(\bar{z} - \bar{z}')/a)\{\exp(2 n \ \delta g(\rho)) - 1\}] \quad (7)$$

with $\rho = r' - r$.

The first term in the bracket is an harmonic which we discard as irrelevant. The second term involves the *difference* $(\bar{z} - \bar{z}')$: it will act to renormalize γ.

For an infinitesimal renormalization, δg is small and we can write

$$\exp(2\,n\,\delta g(\rho)) - 1 \simeq 2\,n\,\delta g(\rho)\,.$$

One could then argue that the range of ρ is small, so that a further expansion is allowed

$$\cos\,(2\,\pi(\bar z - \bar z')/a) \simeq 1 - 2\,\pi^2(\bar z - \bar z)^2/a^2 \simeq$$
$$\simeq 1 - 2\,\pi^2(\rho \cdot \mathrm{grad}\,\bar z)^2/a^2. \quad (8)$$

If we accept (8), the renormalization of γ follows at once :

$$\delta\gamma = (\pi^2/a^2)(n\bar V^2/T)\int \rho^2\,\mathrm{d}^2\rho\;\delta g(\rho)\,. \quad (9)$$

Indeed, that is the procedure followed in many papers on the subject. Unfortunately, (9) is wrong. If we use a sharp cut off Λ, the integral over ρ is identically zero (it involves the integral $\int \bar z\,\delta z\,\mathrm{d}^2 r$, which vanishes since the Fourier components of $\bar z$ and δz are non overlapping). If one uses a smooth cut off that extends down to $k = 0$, the integral is finite. However $\delta\gamma$ is then an *artefact* of the cut off procedure : because the renormalization touches long wave length fluctuations ($k \to 0$), one must correct γ ; but that correction is put by hand and it has nothing to do with mode-mode coupling. (This is especially obvious if one considers an harmonic potential $\mathbf{V} = \varepsilon z^2/2$ instead of the periodic potential used here : the above formulation does yield a $\delta\gamma$, while physically all modes are obviously decoupled).

We are thus forced to two conclusions : (i) a smooth cut off should *not* extend down to $k = 0$ if the renormalization $\delta\gamma$ is to make any sense ; (ii) the expansion (8) is then incorrect, since it would yield $\delta\gamma = 0$: the correct procedure was given by Knops and den Ouden [5]. When handling the factor $\cos\,(2\,\pi(\bar z - \bar z')/a)$ in (7), we should consider that $\bar z$ is the sum of two contributions : the *equilibrium* fluctuations $\bar z_{\rm eq}$, and a small correction ζ in which we are explicitly interested (for instance the response to a small long wave length perturbation). We want to expand with respect to ζ, but *not* with respect to $\bar z_{\rm eq}$. Consequently, we average over $\bar z_{\rm eq}$ before expanding in ζ :

$$\cos\,(2\,\pi(\bar z - \bar z')/a) \to$$
$$\to \langle\cos\,(2\,\pi(\bar z - \bar z')/a)\rangle_{\rm eq}[1 - 2\,\pi^2(\zeta - \zeta')^2/a^2]\,.$$

In analogy with δg, we define

$$\bar g(\rho) = (2\,\pi\gamma/T)\langle\bar z(r)\,\bar z(r + \rho)\rangle =$$
$$= \int_0^\infty (\mathrm{d}k/k)\,J_0(k\rho)(1 - \psi)\,f$$

from which we infer (in lowest order $V = 0$)

$$(\pi\gamma/T)\langle(\bar z - \bar z')^2\rangle = \bar h(\rho) = \bar g(0) - \bar g(\rho) =$$
$$= \int_0^\infty (\mathrm{d}k/k)[1 - J_0(k\rho)](1 - \psi)\,f\,.$$

The erroneous result (9) is then replaced by

$$\delta\gamma = (\pi^2/a^2)(n\bar V^2/T)\,\times$$
$$\times \int \rho^2\,\mathrm{d}^2\rho\;\delta g(\rho)\exp(-2\,n\bar h(\rho)) \quad (10)$$

$\delta\gamma$ is thus controlled by *all* fluctuations, those of $\bar z$ as well as of δz. Note that all divergences have been eliminated, in δg because the region $k = 0$ is excluded, in $\bar h$ because we consider the *difference* $(\bar z(0) - \bar z(\rho))$. (10) is finite and well defined, even for a sharp cut off (the convergence is ensured by the new factor $\exp(-2\,n\bar h)$).

Until now, the form factors f and ψ were left completely open. We now make one further assumption : the renormalization transformation is merely a *change of scale*. In the first stage of renormalization, the cut off is reduced from the original Λ_0 to some value Λ, so that the form factor is the scaled expression $f(k/\Lambda)$. Subsequent renormalization brings Λ to $\bar\Lambda$, so that

$$\bar f = (1 - \psi)\,f = f(k/\bar\Lambda)\,,$$
$$\delta f = \psi f = f(k/\Lambda) - f(k/\bar\Lambda)\,.$$

It is easily verified that

$$\delta g(0) = \int_0^\infty (\mathrm{d}k/k)[f(k/\Lambda) - f(k/\bar\Lambda)] =$$
$$= \mathrm{Log}\,(\Lambda/\bar\Lambda)\,.$$

More generally, all quantities may be expressed in terms of the dimensionless variables $\tilde r = \rho\Lambda$ and $\tilde k = k/\Lambda$. For instance

$$h(\rho) = H(\tilde r) = \int_0^\infty (\mathrm{d}\tilde k/\tilde k)[1 - J_0(\tilde k\tilde r)]\,f(\tilde k)\,. \quad (11)$$

For an infinitesimal transformation, $\bar\Lambda = \Lambda(1 - \varepsilon)$, we have similarly

$$\delta g(\tilde r) = -\varepsilon\int_0^\infty \mathrm{d}\tilde k\,J_0(\tilde k\tilde r)\,f'(\tilde k) = \varepsilon(1 - \tilde r(\mathrm{d}H/\mathrm{d}\tilde r))\,.$$

If we introduce the potential energy $U = V/\Lambda^2$ over a $(1/\Lambda \times 1/\Lambda)$ cell, the *scaled* renormalization equations take the simple form :

$$(\mathrm{d}U/\mathrm{d}\varepsilon) = (2 - n)\,U$$
$$(\mathrm{d}\gamma/\mathrm{d}\varepsilon) = (2\,\pi^4\,U^2/\gamma a^4)\,A(n) \quad (12)$$

in which we have set

$$n = \pi T/\gamma a^2$$
$$A(n) = \int_0^\infty \tilde r^3\,\mathrm{d}\tilde r\,\exp(-2\,nH(\tilde r))(1 - \tilde r(\mathrm{d}H/\mathrm{d}\tilde r))\,.$$

$$(13)$$

The equations (12) are the usual Kosterlitz-Thouless renormalization equations, the only new feature being an *accurate* expression of $A(n)$, valid for arbitrary values of n (i.e. of T) up to second order in U. That improvement will be important when fitting experiments away from T_R [9-10].

Note that (13) holds for an arbitrary form factor f (hidden in H). It is well defined even for a sharp cut off, $f(x) = \theta(1 - x)$.

The renormalization constant $A(n)$ depends on temperature. It may be written as

$$A(n) = (1/2\,n) \int_0^\infty \tilde{r}^{(4 - 2n)} d\tilde{r}(d/d\tilde{r}) \times$$

$$\times \left[\exp(2\,n(\text{Log}\,\tilde{r} - H)) \right]$$

from which we infer at once the value *at the fixed point* $n = 2$:

$$A(2) = (\gamma a^2/2\,\pi T) \exp\left[\lim_{\tilde{r} \to \infty} 4(\text{Log}\,\tilde{r} - H) \right]$$

(at the fixed point, A is controlled by $\tilde{r} \gg 1$). For a sharp cut off, we find

$$A(2) = 4\,e^{-4\,\Gamma} = 0.398$$

(Γ is Euler's constant). The behaviour at $n \neq 2$ will be discussed later, within a slightly different, « dynamic », renormalization scheme : it will be seen that $A(n)$ differs appreciably from its usual approximations.

Our result (12) and (13) differs from those of Minnhagen [11], who also derived renormalization equations away from the fixed point. For instance, our $A(n)$ is smooth, displaying no singularity at a temperature $T^* < T_R$. The origin of that discrepancy is unclear, the two languages being very different. Minnhagen scaling equation for U is non local in the parameter ε, a surprising feature within a first order calculation. In contrast his scaling equation for γ is simple. It may be that his approach includes some of the higher order term ($\sim U^3$), which we do omit. We can only argue that our calculation is systematic to order U^2 : to *that order,* and for our *particular* renormalization scheme, the expression of $A(n)$ is exact.

2. Dynamic renormalization.

Following Chui and Weeks [6], we start from a Langevin equation for the profile fluctuation $z(r, t)$:

$$\eta \, \partial z/\partial t = \gamma \, \nabla^2 z - (2\,\pi V/a) \sin(2\,\pi z/a) + R \quad (14)$$

η is a *friction coefficient,* R a random noise force with a white spectrum

$$\langle R_k(t)\,R_k(t') \rangle = G_k\,\delta(t - t') \,.$$

Note that no mass is attributed to the interface : this

means that any deformation would diffuse rather than propagate along the interface.

In the absence of a periodic potential V, (14) is linear and it yields

$$\langle z_k^2 \rangle = G_k/2\,\eta\,\gamma k^2 \,.$$

In order to reproduce the result of section 1, $\langle z_k^2 \rangle = (T/\gamma k^2)\,f$, we have two possibilities :

(i) either correct the stiffness term γk^2 : that was the choice of section 1.

(ii) or cut off the spectrum of the random force, setting

$$G_k = 2\,\eta T f_k \,.$$

From now on, we adopt the latter philosophy (« modified » fluctuation dissipation theorem), which will result in a slightly different renormalization scheme.

When $V = 0$, the solution of (14) is straightforward

$$z(r, t) = \int_{-\infty}^t dt' \int d^2r'\, \chi_0(r - r', t - t')\,R(r', t') \quad (15)$$

where χ_0 is the diffusion response function

$$\chi_0(r, t) = (1/4\,\pi \gamma t) \exp(-\eta r^2/4\,\gamma t)\,,$$

$$\chi_0(k, t) = (1/\eta)\exp(-\gamma k^2 t/\eta)\,.$$

The distribution of z_k is Gaussian, and the corresponding correlation function is simply

$$g(\rho, \tau) = (2\,\pi \gamma/T)\langle z(r, t)\,z(r + \rho, t + \tau) \rangle =$$

$$= \int_0^\infty (dk/k)\,J_0(k\rho)\exp(-\gamma k^2 \tau/\eta)\,f(k/\Lambda)\,.$$

We can again introduce dimensionless variables, $\rho\Lambda = \tilde{r}$ and $\gamma\tau/\eta\rho^2 = x$: all correlation functions depend on $\tilde{r}$ and x, for instance

$$H(\tilde{r}, x) = g(0, 0) - g(\rho, \tau) = \int_0^\infty (dk/k) \times$$

$$\times [1 - J_0(k\tilde{r})\exp(-k^2 \tilde{r}^2 x)]\,f(k)\,. \quad (16)$$

At large values of $\tilde{r}, \tilde{r} \gg 1$, we can ignore the cut off factor in the second term of (16) : we then find

$$\delta H/\delta x =$$

$$= \int_0^\infty k\,dk\,J_0(k)\exp(-k^2 x) = 2\,\pi\eta\rho^2\chi_0(\rho, \tau) \quad (17)$$

a relationship which we shall use later.

When V is finite, an explicit solution such as (15) is no longer possible. We can solve (14) by *iteration* ; once again the best way is to set up a renormalization scheme. Quite generally, $z(t)$ is a functional of R, $z[R(t')]$. We split R in two parts, $R = \bar{R} + \delta R$ which are statistically independent, such that the resultant

power spectrum G is the sum $(\overline{G} + \delta G)$ of the respective contributions of $\overline{R}$ and δR. We then perform a *partial average* over δR, defining

$$\overline{z} = \langle z[\overline{R} + \delta R]\rangle_{\delta R} \, .$$

As a result of non linearities, the equation of motion for $\overline{z}$ is modified. Note that we eliminate a piece of the *random force* R, and not of the fluctuations z_k, as in section 1 : beyond a linear approximation, the two schemes are different, as we shall see shortly. Setting $\delta z = z - \overline{z}$, we obtain two equations of motion

$$\eta\,(\partial\overline{z}/\partial t) = \gamma\,\nabla^2\overline{z} + \overline{R} - (2\,\pi V/a) \times$$
$$\times\,\langle\sin\,(2\,\pi(\overline{z} + \delta z)/a)\rangle \quad (18)$$

$$\eta\,(\partial(\delta z)/\partial t) = \gamma\,\nabla^2(\delta z) + \delta R - (2\,\pi V/a) \times$$
$$\times\,\{\sin\,(2\,\pi(\overline{z} + \delta z)/a) - \langle\sin\,(2\,\pi(\overline{z} + \delta z)/a)\rangle\}\,.$$

We solve for δz by iteration, expanding in powers of V.

In zeroth order

$$\delta z^{(0)}(r,t) = \int d^2r'\,dt'\,\chi_0(r - r', t - t')\,\delta R(r', t')$$

where δR is characterized by its power spectrum

$$\langle\delta R_k(t)\,\delta R_k(t')\rangle =$$
$$= \delta\,(t - t')\,\delta G_k = 2\,\eta T\psi f\,\delta\,(t - t')$$

(notations are similar to section 1). In first order

$$\delta r^{(1)}(r,t) = (-2\,\pi V/a) \times$$
$$\times\int d^2r'\,dt'\,\chi_0(r - r', t - t')$$
$$\times\,\{\sin\,(2\,\pi(\overline{z} + \delta z^{(0)})/a)$$
$$- \langle\sin\,(2\,\pi(\overline{z} + \delta z^{(0)})/a)\rangle\}\,.$$

We carry the resulting δz into the equation of $\overline{z}$, and we perform the average. We thus find, to order V^2

$$\eta\,(\partial\overline{z}/\partial t) = \gamma\,\nabla^2\overline{z} + \overline{R} - (2\,\pi\overline{V}/a)\sin\,(2\,\pi\overline{z}/a) + (4\,\pi^3\overline{V}^2/a^3)\int d^2\rho\,d\tau\chi_0(\rho,\tau)\times$$

$$\times\,\{\sin\,(2\,\pi(\overline{z}(r,t) + \overline{z}(r + \rho, t + \tau))/a)[\exp(-2n\,\delta g(\rho,\tau)) - 1]$$
$$+ \sin\,(2\,\pi(\overline{z}(r,t) - \overline{z}(r + \rho, t + \tau))/a)[\exp(+2n\,\delta g(\rho,\tau)) - 1]\} \quad\quad\quad (19)$$

$\delta g(\rho,\tau)$ is the correlation function of $\delta z^{(0)}$ (here, it is retarded).

$\overline{V} = V\exp[-n\,\delta g(0,0)]$ is the new periodic potential reduced by fluctuations, as in section 1. As it stands, (19) is still exact to order V^2.

We now introduce approximations. In the bracket of (19), we discard the first term as an irrelevant harmonic. In the second term, we follow the same course as in section 1 : $\overline{z}$ is the sum of an *equilibrium* fluctuation (over which we average), and of a *slowly varying* part which we follow explicitly (for instance the response to an external probe). We thus make the replacement

$$\sin\,(2\,\pi(\overline{z} - \overline{z}')/a)$$
$$\rightarrow 2\,\pi(\overline{z} - \overline{z}')/a\,\langle\cos\,(2\,\pi(\overline{z} - \overline{z}')/a)\rangle_{\overline{R}}$$

where $\langle\ \rangle_{\overline{R}}$ is an average over *large scale* fluctuations. (In a simple minded expansion, this last factor would be missing). When Taylor expanding $(\overline{z} - \overline{z}')$, the $\nabla^2\overline{z}$ term acts to renormalize γ, the $\partial\overline{z}/\partial t$ term corrects η. For an infinitesimal transformation (δg : small), we thus find

$$\Delta\gamma = (4\,\pi^4/a^4)\,n\overline{V}^2\iint \rho^2\,d^2\rho\int_0^\infty d\tau\,\chi_0(\rho,\tau)\times$$
$$\times\exp(-2nh(\rho,\tau))\,\delta g(\rho,\tau)$$

$$\Delta\eta = (16\,\pi^4/a^4)\,n\overline{V}^2\iint d^2\rho\int_0^\infty \tau\,d\tau\,\chi_0(\rho,\tau)\times$$
$$\times\exp(-2nh(\rho,\tau))\,\delta g(\rho,\tau) \quad (20)$$

in which h and δg are the retarded versions of our previous static quantities. (20) replaces our former static result (10).

We did not specify yet the new form factor $\overline{f} = (1 - \psi)\,f$: again, we choose it so that the spectrum of $\overline{R}$ is deduced from that of R by a simple change of *scale*, $\Lambda \rightarrow \overline{\Lambda}$. As in section 1, everything may then be cast in dimensionless variables, $\tilde{r}$ and x. Using our explicit expression for χ_0, we obtain the following final set of equations for an *infinitesimal scaling transformation* :

$$(dU/d\varepsilon) = (2 - n)\,U$$

$$(d\gamma/d\varepsilon) = (2\,n\pi^4\,U^2/\gamma a^4)\int_0^\infty \tilde{r}^3\,d\tilde{r}\int_0^\infty (dx/x)\times$$
$$\times e^{-1/4\,x}\,e^{-2nH}[d\,\delta g/d\varepsilon] = (2\,\pi^4\,U^2/\gamma a^4)\,A(n)$$

$$(d\eta/d\varepsilon) = (8\,n\pi^4\,U^2\,\eta/\gamma a^4)\int_0^\infty \tilde{r}^3\,d\tilde{r}\int_0^\infty dx\,e^{-1/4\,x}$$
$$\times e^{-2nH}[d\,\delta g/d\varepsilon] = (8\,\pi^4\,U^2/\gamma a^4)(\eta/\gamma)\,B(n)$$
$$(21)$$

in which we have set

$$n = (\pi T/\gamma a^2)\,,$$
$$[d(\delta g)/d\varepsilon](\tilde{r}, x) = J_0(\tilde{r})\times\exp(-\tilde{r}^2 x)\,, \quad (22)$$
$$U = V/\Lambda^2$$

$$H(\tilde{r}, x) = \int_0^1 (dk/k)[1 - J_0(k\tilde{r})\exp(-k^2\tilde{r}^2 x)]\,.$$

(We again assume a sharp cut off, $f(x) = \theta(1-x)$). (21) and (22) constitute the basic result of our dynamical scaling theory. Within second order in U, the equations are exact : we do not use any « long time » approximation in evaluating the coefficients $A(n)$, $B(n)$, which are well defined for arbitrary values of n (i.e. of the temperature). Note that the x integration (« time ») guarantees convergence.

At this stage, two questions arise :

(i) To what extent is the dynamical result (21) equivalent to our former static result (13) ?

(ii) How does (21) compare with the former result of Chui and Weeks [3] ?

In order to answer point (i), we note that

$$[d(\delta g)/d\varepsilon](\tilde{r}, x) = 1 - \tilde{r}[\delta H(\tilde{r}, x)/\partial\tilde{r}]$$

(a relation which follows from (22)). Integrating by part over $\tilde{r}$, we may cast $A(n)$ in the form

$$A(n) = (n - 2) \int_0^\infty \tilde{r}^3 \, d\tilde{r} \int_0^\infty (dx/x) \, e^{-1/4\,x} \, e^{-2\,nH}$$

$$(23)$$

(to the extent that (23) converges, i.e. if $n \geqslant 2$). At the fixed point $n = 2$, the integral (23) is dominated by *large* values of $\tilde{r}$, for which the approximate result (17) holds. In our reduced units, that means

$$\partial H(\tilde{r}, x)/\partial x = e^{-1/4\,x}/2\,x .$$

The integration over x is then obvious, yielding

$$\int_0^\infty dx/x \, e^{-1/4\,x} \, e^{-2\,nH} = (1/n)[e^{-2\,nH}]_\infty^0 =$$

$$= (1/n) \exp(-2\,nH(\tilde{r}, 0)) .$$

In comparison, the static result (13) may be written as

$$A(n) = ((n - 2)/n) \int_0^\infty \tilde{r}^3 \, d\tilde{r} \exp(-2\,nH(\tilde{r}, 0))$$

(we integrate by parts over $\tilde{r}$). We conclude that the *static and dynamical calculations of A are identical at the fixed point $n = 2$*. This result was expected since the behaviour at the fixed point is universal.

Away from the fixed point, the equivalence no longer holds (integrals are *not* dominated by large $\tilde{r}$). This result was also expected, since we use different schemes in eliminating short wavelength fluctuations (cutting off z_k in one case, the random force R_k in the other). In what follows, we shall prefer the dynamical result (23), partly because it is based on a more intuitive cut off scheme, partly because it allows a systematic *joint* treatment of η and γ, summarized in the dimensionless equation

$$(d\eta/d\gamma) = (\eta/\gamma) \, C(n)$$

with $C = 4\,B/A$.

In order to construct the scaling trajectories, we must know the functions $A(n)$ and $B(n)$ (which are usually approximated by their fixed point values at $n = 2$). At the fixed point itself, we know from our static calculation that $A(2) = 4 \, e^{-4\,\Gamma} = 0.398$. A numerical integration yields $C(2) = 2.35$. For *high* temperatures, $n \gg 2$, the integrals in (21) are dominated by small values of $\tilde{r}$, and we may expand H and δg. The results are expressed in terms of the exponential integral

$$Ei(-x) = \int_\infty^x e^{-t}(dt/t) .$$

When $n \to \infty$,

$$A(n) \simeq (8/n)[-1 - 2\,eEi(-1)] = 1.54/n$$

$$B(n) \simeq (2/n)[1 + eEi(-1)] = 0.807/n$$

$$C(n) \simeq 2.09 .$$

At *low* temperatures, $n \to 0$, we may set $e^{-2\,nH} = 1$: we then find $A(n) \sim n^2$, $B(n) = (n/2) + 0(n^2)$. In between, we integrated (21) numerically : the results are shown in figures 1 to 3. We note that the renormalization of γ and η disappears at low and high n (i.e. $T \ll T_R$ and $T \gg T_R$).

One may rightly question the relevance of these results below $T_R (n < 2)$. For a flat interface in equilibrium, we know that U blows up when the length scale exceeds the correlation length : the expansion in powers of U is then meaningless, and the precise behaviour of $A(n)$, $B(n)$ does not matter much. However we shall see shortly that one may have to *interrupt* renormalization at some *finite* length scale, either because the interface is tilted or because it is growing. Even if

$T < T_R$, it may happen that U is still small when scaling stops, in which case the second order equation (21) remains valid : $A(n)$ and $B(n)$ are then physically meaningful, despite the fact that $n < 2$.

In their basic paper, Chui and Weeks [6] also calculated the coefficients A, B, C. Their results are shown in figures 1-3. As regards A and B, the comparison is only qualitative, since their definition of the renormalized potential U is somewhat ambiguous. On the other hand, there is no ambiguity in the *ratio* $C(n)$: the two calculations clearly disagree. Chui and Weeks find a divergence of C (and B) at $n = 1$, which does not appear in our more accurate expansion to order U^2. From a purely technical point of view, such a discrepancy probably arises from their use of a *logarith-*
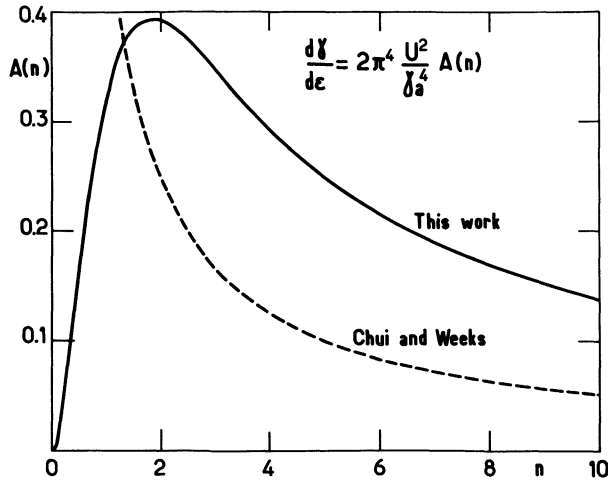
Fig. 1. — The constant $A(n)$ as a function of $n = (\pi T/\gamma a^2)$. The full line is our result obtained from (21). The dashed line is an estimate from Chui and Weeks calculation.
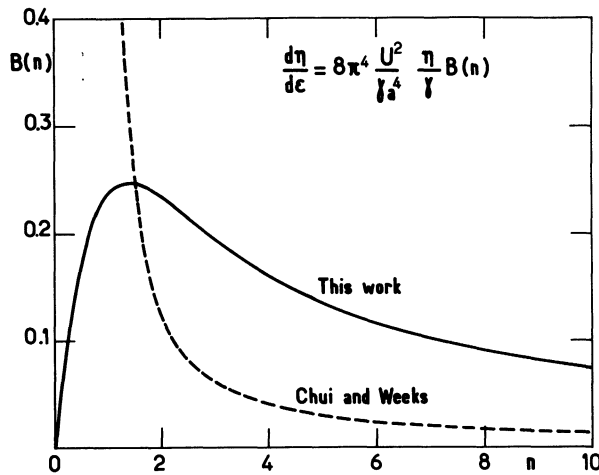

Fig. 2. — Same data as in figure 1, for the coefficient $B(n)$ that controls the renormalization of the friction coefficient η.
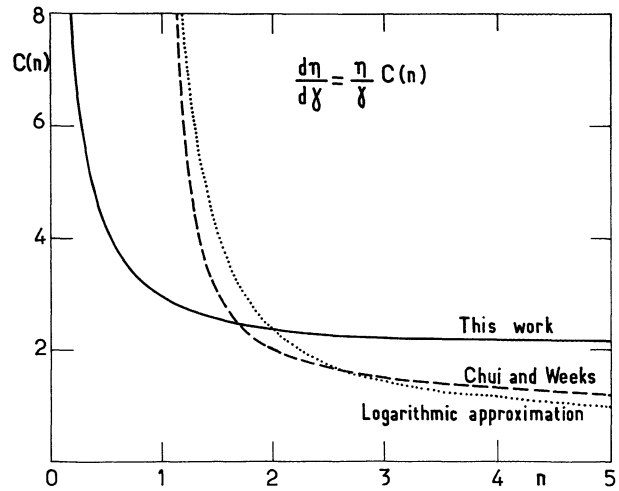

Fig. 3. — The coefficient $C(n) = (\gamma/\eta)(\mathrm{d}\eta/\mathrm{d}\gamma)$. The full line is our result deduced from (21). The dashed line is the result of Chui and Weeks. The dotted line corresponds to a « logarithmic » approximation to our accurate result, based on the asymptotic behaviour of correlation functions. Note that the full and dotted lines cross at the fixed point $n = 2$, where the logarithmic approximation is valid.

mic approximation (common in such problems), in which all correlation functions are replaced by their long time τ, long length ρ asymptotic behaviour (at least, it is our guess, as their paper does not give much detail on the way the calculation is handled). We saw that such an approximation, while valid at the fixed point, was definitely wrong for $n \neq 2$. Indeed, let us assume that the relation (17), valid for large $\tilde{r}$, holds everywhere. We may then integrate it to obtain

$$H(\tilde{r}, x) = H(\tilde{r}, 0) - (1/2)\,Ei(-1/4\,x) \qquad (24)$$

Integrating (21) by parts over ρ, we may write
$[\mathrm{d}\eta/\mathrm{d}\gamma] =$

$$= [4\,\eta/\gamma]\frac{\displaystyle\int_0^\infty \tilde{r}^3\,\mathrm{d}\tilde{r}\int_0^\infty \mathrm{d}x\,\mathrm{e}^{-1/4\,x}\,\mathrm{e}^{-2\,nH}}{\displaystyle\int_0^\infty \tilde{r}^3\,\mathrm{d}\tilde{r}\int_0^\infty (\mathrm{d}x/x)\,\mathrm{e}^{-1/4\,x}\,\mathrm{e}^{-2\,nH}}.$$

In view of (24), the integrals over x and ρ separate out, and we obtain

$$C(n) = 4\,\frac{\displaystyle\int_0^\infty \mathrm{d}x\,\mathrm{e}^{-1/4\,x}\exp(nEi(-1/4\,x))}{\displaystyle\int_0^\infty (\mathrm{d}x/x)\,\mathrm{e}^{-1/4\,x}\exp(nEi(-1/4\,x))}.$$

The numerator must be calculated numerically. The resulting C is also displayed in figure 3 : it resembles the result of Chui and Weeks (it also diverges at $n = 1$), but it is drastically different from the actual $C(n)$. We thus conclude that logarithmic approximations must be used with caution. Away from the fixed point, an accurate calculation of the scaling coefficients A and B is essential : that is why we discussed our renormalization scheme in great detail.

At this stage, it may be useful to put our calculation of A, B, C in perspective. Strictly speaking, a renormalization scheme is universal only at T_R : away from the transition, different schemes lead to different intermediate results in the scaling process (our static and dynamic approaches provide a specific example). Thus, it is not surprising that our results and those of Chui and Weeks should differ (although the slight difference of $C(n)$ at the fixed point $n = 2$ should not be there : the origin of that discrepancy is unclear). In their paper, Chui and Weeks were concerned with a flat interface near equilibrium, for which scaling proceeds to the end : their result is meant to apply only when $T \geqslant T_R$, a region in which our results are similar. Here, we shall also exploit the scaling equations below T_R : we then need a more accurate determination of A, B, C — admittedly non-universal, but exact within a

well defined renormalization scheme. In this way, we may hope to obtain reasonable results, albeit approximate since the scaling process is not unique. While essential quantitatively, such an improvement does not modify the main qualitative conclusions of Chui and Weeks.

Once we know $A(n)$ and $B(n)$, the scaling trajectories are easily deduced from (21). In the (U, γ) plane, they are the usual Kosterlitz Thouless hyperbolae near the fixed point. Away from $n = 2$, they depart from that shape, even to order U^2: the corrections are significant in order to compare with experiments. Indeed, such corrections considerably improve the theoretical fit of curvature and step energy measurements. The numerical integration of (21) is shown in figure 4, using our exact result for $A(n)$.
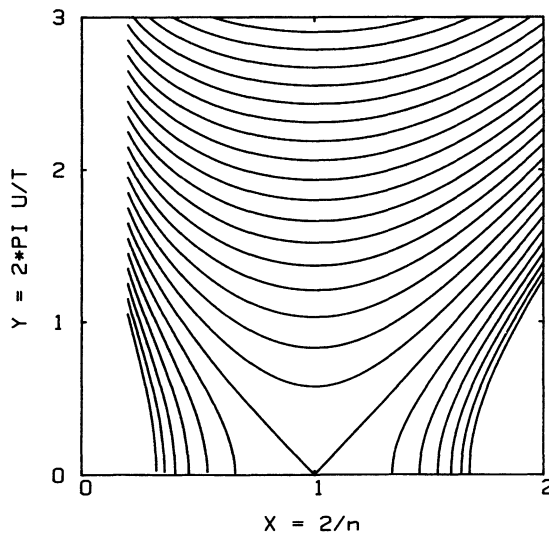
Fig. 4. — Renormalization trajectories in the $(X = 2/n,$ $Y = 2 \pi U/T)$ plane, using our exact expression of $A(n)$.

3. Vicinal surfaces : interrupted renormalization.

Until now, we only considered an average interface parallel to the crystal planes. We now extend our argument to a *vicinal* surface, making a small angle θ with the crystal planes. We still ignore anisotropy around the crystal axis, as well as « in plane » periodicity : our crystal is a stack of isotropic plates.

The surface *energy* $\alpha(\theta)$ depends on orientation : if the surface fluctuates by a small additional $z(r)$ (grad $z = \theta'$), the surface energy has the form

$$E = \int \alpha(|\theta + \theta'|)(1 + \theta'^2)^{1/2} \, d^2r =$$

$$= E_0 + \int d^2r(\beta_i \, \theta'_i + 1/2 \, \gamma_{ij} \, \theta'_i \, \theta'_j + \cdots)$$

β_i only has a *longitudinal* component (along the projection of the crystal axis on the average surface).

$$\beta_\| = \partial\alpha/\partial\theta . \tag{24'}$$

For an interface which is fixed at the ends, the corresponding term in the energy integrates to zero. Similarly, γ has different longitudinal and transverse components :

$$\gamma_\| = \alpha + (\partial^2\alpha/\partial\theta^2),$$
$$\gamma_\perp = \alpha \xi + (1/\theta)(\partial\alpha/\partial\theta). \tag{25}$$

The term α arises from surface *stretching* (*via* the factor $(1 + \theta'^2)^{1/2}$), the second term is due to surface *rotation*. From γ_{ij}, we infer the thermal equilibrium fluctuations

$$\langle z_k^2 \rangle = T/(\gamma_{ij} \, k_i \, k_j) \Rightarrow \langle z^2 \rangle =$$

$$= T/(2 \, \pi(\gamma_\| \gamma_\perp)^{1/2}) \int dk/k .$$

In our former scaling relations, γ will thus be replaced by the average $(\gamma_\| \gamma_\perp)^{1/2}$ — namely

$$n = \pi T/(a^2(\gamma_\| \gamma_\perp)^{1/2}).$$

From this brief discussion, it is clear that all the physical information is contained in $\alpha(\theta)$.

When $T > T_R$, $\alpha(\theta)$ is an analytic function of θ. Below the roughening transition, $\alpha(\theta)$ displays a singular cusp at $\theta = 0$, resulting in the formation of facets : we want to understand this crossover by extending our renormalization scheme to a tilted interface. Rather than tilting the interface, we tilt the crystal planes : the equilibrium profile is still $z = 0$, but the periodic potential is now $- V \cos(2 \pi(z + \theta x)/a)$. (A similar approach was used by Horowitz *et al.* [4]). The calculation is essentially the same as before, but for the replacement of z by $(z + \theta x)$ everywhere. It can be done either in the static or in the dynamic version : we first try the static one.

In first order, the scaling equation (12) for U is unchanged, but for the refined expression of n (actually, the anisotropy of γ is of order V^2: it will not affect much the scaling trajectoires). In second order, we again discard the harmonic contribution. The remaining « effective » second order energy is similar to (7).

$$E^{(2)} = (- \overline{V}^2/4 \, T) \iint d^2r \, d^2r' \times$$

$$\times \cos(2 \, \pi(\overline{z} - \overline{z}' + \theta\rho_x)/a)$$
$$\times (\exp(2 \, n \, \delta g(\rho)) - 1) \tag{26}$$

(where ρ_x is the component of $\boldsymbol{\rho} = \mathbf{r}' - \mathbf{r}$ along the tilt axis). Again, we assume that $\overline{z}$ is the sum of an equilibrium fluctuation $\overline{z}_{eq}$ (over which we average) and a small slowly varying perturbation ζ (which can be expanded). In zeroth order in ζ, (26) generates directly the surface energy $\alpha(\theta)$, which in an infinitesimal renormalization $(V \simeq \overline{V})$ acquires a contribution :

$$\delta\alpha(\theta) = (- \pi V^2/2 \, \gamma a^2) \int d^2\rho \, \delta g(\rho) \times$$

$$\times \exp(- 2 \, nh(\rho)) \cos(2 \, \pi\theta\rho_x/a) . \tag{27}$$

(The tilt only enters through the extra factor $\cos (2 \pi \theta p_x/a)$. Similarly, the terms of order ζ and ζ^2 generate the stress coefficients β_i and γ_{ij} :

$$\delta \beta_i = (\pi^2 V^2/\gamma a^3) \int d^2\rho \ \rho_i \ \delta g(\rho) \times$$

$$\times \exp(- 2 nh(\rho)) \sin (2 \pi \theta p_x/a)$$

$$\delta \gamma_{ij} = (2 \pi^3 V^2/\gamma a^4) \int d^2\rho \ \rho_i \ \rho_j \ \delta g(\rho) \times$$

$$\times \exp(- 2 nh(\rho)) \cos (2 \pi \theta p_x/a) . \quad (28)$$

We could equally well carry the renormalization in a dynamic language : we would thus recover the scaling equations (21), with an extra kernel $K(2 \pi \theta \bar{r}/a\Lambda)$ in the integral, with

$$K(u) = \begin{cases} \langle 2 \cos^2 \varphi \cos [u \cos \varphi] \rangle_\varphi = 2 J_1'(u) & \text{for } \gamma_{\parallel} \\ \langle 2 \sin^2 \varphi \cos [u \cos \varphi] \rangle_\varphi = 2 J_1(u)/u & \text{for } \gamma_{\perp} \\ \langle \cos [u \cos \varphi] \rangle_\varphi = J_0(u) & \text{for } \eta. \end{cases}$$

(φ is the azimuthal angle of ρ).

From (27) and (28), it is easily verified that

$$\delta \beta_{\parallel} = d\delta\alpha/d\theta, \quad \delta \gamma_{\parallel} = d^2\delta\alpha/d\theta^2,$$

$$\delta \gamma_{\perp} = (1/\theta) d\beta_{\parallel} = (1/\theta) d\delta\alpha/d\theta .$$

We thus recover the thermodynamic identities (25), but for one point : we have lost the « stretching » contribution $\alpha \delta_{ij}$ to the surface stress tensor. The error arises from the replacement of $(1 + \theta'^2)^{1/2}$ by $1 + \theta'^2/2$ at the beginning of our calculation. Higher order terms are indeed negligible if they multiply $(\text{grad } \bar{z})^2$, but they are not in a zeroth order contribution such as (27). More specifically, a slope $\theta' = \text{grad } \bar{z}$ will modify the thermal average of $\langle \delta z^2 \rangle$, hence the second order energy (26) and ultimately the stress $\gamma \sim \partial^2 E/\partial \theta'^2$. A detailed analysis yields the exact identities (25), as expected.

Of course, thermal fluctuations are controlled by the total γ_{ij}, including the stretching part of $\alpha \delta_{ij}$: strictly speaking, our former renormalization scheme is thus incorrect. However, the error is only significant in the initial stages of the scaling process. Comparing (27) and (28), we see that the ratio $\delta\gamma/\delta\alpha$ is $\sim (\rho/a)^2 \sim 1/(\Lambda a)^2$. The stretching contribution to γ is thus sizeable only if $a\Lambda \sim 1$, a condition which is indeed met at the microscopic level. On the other hand, Λ is smaller and smaller as scaling proceeds : the « stretching » contribution to $\delta\gamma$ quickly becomes irrelevant. It does not affect the universal Kosterlitz-Thouless behaviour near the fixed point. It only acts in the initial « transient » stages of renormalization to correct the quantitative value of γ. Since the initial parameters of our model are largely adjustable, we shall ignore such corrections. We use (28) for γ_{ij}, disregarding the small stretching term. As a result

$$\gamma_{\parallel} \simeq (d/d\theta)(\theta \gamma_{\perp}) = \gamma_{\perp} + \theta(\partial\gamma_{\perp}/\partial\theta) \quad (29)$$

a simple relationship which we shall use later.

As seen in (28), the problem now has two length scales, a cut off Λ^{-1} which we are progressively increasing, and the quantity $d = a/\theta$ which corresponds to the distance between crystal steps. As long as $\Lambda d \gg 1$, the effect of the tilt is negligible (the cos in (28) is ~ 1). On the other hand, when $\Lambda d \ll 1$, the integrals over ρ are cut off by the tilt factor : then,

$$\delta\gamma \sim V^2 d^4(\delta\Lambda/\Lambda)$$

$$\delta V/V = n(\delta\Lambda/\Lambda)$$

V keeps decreasing, while the scaling of γ essentially stops (note that $\delta\gamma$ involves V^2 rather than $U^2 = (V/\Lambda)^2$: it does not matter whether $n >$ or < 2).

Rather than using the exact expressions (28), a simple minded approximation is the following :

(i) we integrate the scaling equation with no tilt ($\theta = 0$) from the original Λ_0 up to $\Lambda \sim d^{-1} = \theta/a$.

(ii) We stop scaling there : γ and η depend on θ through the final scale Λ.

Such an approximation only has logarithmic accuracy. Indeed the cut off $\Lambda \sim d^{-1}$ must be different for $\gamma_{\parallel}$ and $\gamma_{\perp}$ in order to achieve the anisotropy predicted in (29) : renormalization stops earlier for $\gamma_{\parallel}$ than for $\gamma_{\perp}$. In order to obtain consistent results, we must estimate one of the γ's — say $\gamma_{\perp}$ — and deduce the other from (29) :

$$\gamma_{\parallel} = \gamma_{\perp} - (d\gamma_{\perp}/dl)$$

where $l = \text{Log} (\Lambda_0/\Lambda) \sim \text{Log} (1/\theta)$. With that word of caution, the « stopped renormalization » method is reasonable as long as the scaling equations are valid, i.e. when U is small.

When $T \geq T_R$, U scales down to zero : the renormalization approach is always valid, yielding a rough interface whose γ and η depend on angle θ. That dependence is obtained by integrating the fundamental scaling equations (12) or (21). Since the calculation was done elsewhere [7], we only quote the main results, assuming for simplicity that $A(n)$ is constant.

(i) The scaling equations have a first integral

$$[\gamma - (\pi T/2 a^2)]^2 - \pi^4(AU^2/a^4) = \text{Const.} , \quad (30)$$

the constant being fixed by the initial values U_0, γ_0. The strength of the pinning potential is measured by the dimensionless coupling constant $t_c = 2 \pi^2 U_0\sqrt{A}/\gamma_0 a^2$.

(ii) At the transition

$$T = T_R(\simeq 2 a^2 \gamma_0(1 + t_c/2)/\pi) ,$$

the surface stiffness is :

$$\gamma(l) = \gamma_0[1 + (t_c^2 l/2(1 + t_c l))] . \quad (31)$$

It goes smoothly from the bare γ_0 at large angles to the

universal value $\gamma_R = \pi T_R/2\, a^2$ when $\theta = 0$. The approach to γ_R is very slow (logarithmic in θ).

(iii) When $T > T_R$, the reduced temperature $t = |T - T_R|/T_R$ should be compared to t_c. At zero angle ($l \to \infty$), the surface stiffness is

$$\gamma_\infty = \gamma_0 \left(1 + \frac{t_c^2}{2\, t_c + 4\, t + 4(t^2 + t t_c)^{1/2}} \right)$$

(it is isotropic). At finite tilt, γ approaches γ_∞ as a power law of angle, $(\gamma_\infty - \gamma) \sim \theta^{4\sigma}$, with $\sigma \sim t$ if $t \ll t_c$, or $\sigma \sim (t t_c)^{1/2}$ if $t \gg t_c$. The angle scale is logarithmic, and γ varies *very slowly*.

In the opposite limit $T < T_R$, the scaling calculation is no longer valid when $U \sim T$, i.e. $\Lambda \sim \xi^{-1}$, where ξ is the *correlation length* of the surface, as given by reference [7] :

$$\text{Log } (\xi/a) \sim \begin{cases} (\pi/2)(t t_c)^{-1/2} & \text{if } t \ll t_c \\[2mm] (1/2\, t)\, \text{Log } (4\, t/t_c) & \text{if } t \gg t_c \,. \end{cases}$$

For a *tilted* interface, $\theta = a/d$, two cases are possible :

(i) Large angles, $\theta \gg a/\xi$: scaling stops *before* the trajectory has diverged, the renormalization approach is valid. The surface *remains rough*, even though $T < T_R$. Physically, that regime corresponds to a distance d between steps much smaller than their width ξ : the *steps overlap* and are no longer identifiable. The surface behaves as if it were rough. (Put another way, a finite tilt θ blurs the transition).

(ii) Small angles, $\theta \ll a/\xi$: scaling then breaks down for $\Lambda\xi \sim 1$. The surface breaks into *discrete steps*, with a width $\sim \xi$ and an energy per unit length $\beta \sim \gamma a^2/\xi$.

In between, there is a crossover region, in which $\gamma_\parallel$ and $\gamma_\perp$ are *universal functions of a single parameter* $\theta\xi/a$. We can only approach these functions from both ends.

Let us first consider the « rough » side of the crossover, $\theta\xi \gg a$. As θ decreases, $\gamma_\parallel$ and $\gamma_\perp$ *increase*, with $\gamma_\perp > \gamma_\parallel$ in view of (29). Since γ will eventually depart appreciably from γ_R, one must take account of the n-dependence of A in writing the first integral (30), which becomes (for T close to T_R) :

$$\int_{\gamma_R}^{\gamma} \mathrm{d}\gamma'(\gamma' - \gamma_R)/A(\pi T/\gamma'\, a^2) = \pi^4\, U^2/2\, a^4\,.$$

In principle, one may infer from this relation a differential equation for $\gamma\,(l)$, yielding the angular dependence $\gamma(\theta)$. Since the expansion in powers of U breaks down, such a calculation makes little sense. Only one feature is sure : in the « scaling region », $\gamma_\parallel$ and $\gamma_\perp$ *increase* when θ goes down.

In the opposite limit $\theta\xi \ll a$, the interface is best

described in terms of a step density n_s per unit length *along the crystal planes*,

$$n_s = 1/d = (\tan \theta)/a \simeq \theta/a\,.$$

The energy per unit area (of crystal plane) is [8]

$$E(n_s) = E_0 + \beta n_s + \Phi n_s^3$$

where E_0 is the reference surface energy of a facet ($\theta = 0$), βn_s the energy of individual steps, Φn_s^3 their interaction resulting for a pair interaction energy Φ/d^2. Within our Sine-Gordon model, Φ results from the confinement of step fluctuations by their neighbours (in real crystals, there exists also an elastic interaction *via* the strain of the underlying crystal which has the same $1/d^2$ dependence). In order to estimate Φ, consider the transverse thermal fluctuations of a single step

$$\langle \delta x^2 \rangle = \sum_q (T/\beta q^2) = (T/\pi\beta) \int_{q_{min}}^{q_{max}} \mathrm{d}q/q^2\,.$$

Since $\langle \delta x^2 \rangle$ is confined to a range $\sim d^2$, all long wave length fluctuations are frozen, with $q_{min} \sim T/\pi\beta d^2$. Each frozen mode costs a free energy $\sim (- T)$, hence a repulsive interaction energy (per unit length)

$$T q_{min}/\pi \sim (T^2/\pi^2\, \beta d^2)\,.$$

As expected, the interaction varies as $1/d^2$, and $\Phi \sim (T^2/\pi^2\, \beta)$.

From $E(n_s)$, one infers the surface energy per unit *interface* area, $\alpha = \cos \theta E(n_s)$, and finally the surface stiffness.

$$\gamma_\parallel = \alpha + \mathrm{d}^2\alpha/\mathrm{d}\theta^2 = E''(n_s)/(a^2 \cos^3 \theta) \simeq 6\, \Phi\theta/a^3$$

$$\gamma_\perp = \alpha + (1/\tan \theta)\, \mathrm{d}\alpha/\mathrm{d}\theta =$$
$$= E'(n_s)/(a \sin \theta) \simeq (\beta/a\theta)\,. \quad (32)$$

The physical interpretation of (32) is simple. $\gamma_\parallel$ corresponds to a fluctuation wave vector perpendicular to the steps, hence to a *step compression* (the steps remain straight) : $\gamma_\parallel$ is controlled by the step compressibility $E''(n)$, as expected. In contrast, $\gamma_\perp$ involves a wave vector parallel to the steps, hence a *step wiggling* (d being unchanged) : $\gamma_\perp$ results from step stretching

$$\left. \begin{array}{l} \partial z/\partial y = n_s a\, \partial x/\partial y \\[1mm] E = (1/2)\, n_s \beta\, (\partial x/\partial y)^2 \end{array} \right\} \Rightarrow \gamma_\perp = \beta/(n_s a^2)\,.$$

We recover (32). The net interface fluctuations involve the combination

$$\bar\gamma = (\gamma_\parallel \gamma_\perp)^{1/2} = (6\, \beta\, \Phi/a^4)^{1/2}\,.$$

In the vicinity of $T_R = 2\, \gamma a^2/\pi$, $\bar\gamma$ is of order γ : *the fluctuations of a vicinal surface are comparable to those of a free surface*, despite the fact that the fluctuation

mechanisms are completely different. The scarcity of steps is compensated by their very large transverse fluctuations (assuming of course that the steps are not pinned by the in plane periodicity).

From (32), we infer the qualitative behaviour of $\gamma_\parallel$ and $\gamma_\perp$ as a function of the universal variable $s = \theta\xi/a$, shown in figure 5. For $s > 1$, the behaviour is logarithmic, while for $s < 1$ we have $\gamma_\parallel \sim \gamma^*s$, $\gamma_\perp \sim \gamma^*/s$. Within our formulation, we cannot characterize the crossover more accurately.

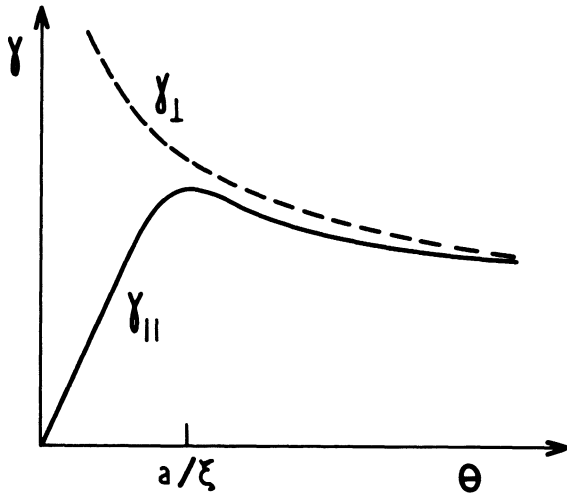Fig. 5. — A sketch of the longitudinal and transverse coefficients $\gamma_\parallel$ and $\gamma_\perp$ as a function of the tilt angle θ. The crossover occurs when the universal parameter $\theta\xi/a$ is of order of 1.

$\gamma_\parallel(\theta)$ and $\gamma_\perp(\theta)$ determine the equilibrium profile of the interface under an applied over pressure δp. Let us define

$$F = \rho_s(\mu_L - \mu_s) = \delta p((\rho_s - \rho_L)/\rho_L) .$$

(Fa is the force on a single step per unit length). For a cylindrical geometry the equilibrium profile $\theta(r)$ is governed by Laplace's law :

$$\gamma_\parallel \cos\theta(d\theta/dr) + \gamma_\perp \sin\theta/r = F . \qquad (33)$$

(In a step regime, $\theta\xi/a \ll 1$, (33) may be interpreted as a mechanical equilibrium of steps, under the combined action of F, step repulsion and step line tension [8]). Using the exact identity $\gamma_\parallel = \gamma_\perp + \tan\theta \, d\gamma_\perp/d\theta$, (33) implies

$$\sin\theta/r = (F/2 \, \gamma_\perp(\theta)). \qquad (34)$$

The measured profile thus gives access to $\gamma_\perp(\theta)$. Below T_R, a flat facet appears, with a radius $R^* = 2\beta/Fa$ which follows from (32) and (34). ($R^*/2$ is the collapse radius at which line tension overcomes the applied force F).

It should be realized however that (33) implies a *local* relationship between γ and θ, a condition which breaks down if the relevant length scale is small compared to the step distance $d = n_s^{-1}$. Near the facet edge, that distance is of order $(\Phi/\beta)^{1/2} \sim \xi$: the very concept of a facet is thus meaningful only if $R^* > \xi$, a rather obvious statement (the « edge » of the facet has width ξ). At a given temperature, there exists a characteristic force

$$F^* \sim (\beta/a\xi) \sim \gamma a/\xi^2 . \qquad (35)$$

When $F \ll F^*$, the facet is large and well defined. When $F \geq F^*$, the edge step spreads to the centre and the facet disappears. We conclude that the *roughening transition is blurred under an applied force F*. Facetting appears *progressively* at a temperature $T < T_R$ such that $\xi(T) \sim (\gamma a/F)^{1/2}$. Above that temperature, the interface *looks rough*, despite the fact that $T < T_R$.

This important conclusion can also be reached within our renormalization scheme. Under the applied force F, a *free* interface acquires a curvature radius $R_i \sim 2\gamma/F$. A surface element of width L thus *bulges*, with a vertical displacement $\zeta \sim L^2/R_i$; this *average* displacement is superimposed on the short wavelength $(kL < 1)$ thermal fluctuations. Two cases are then possible.

(i) $\zeta \ll a$, i.e. small scales $L \ll (aR_i)^{1/2}$: the bulge is unimportant, and the surface element fluctuates as if F was zero.

(ii) $\zeta \gg a$: the bulge averages the periodic potential V to zero, even in the absence of thermal fluctuations. The surface behaves as if it were free.

We are thus led *to stop renormalization* at a characteristic scale $L^* = 1/\Lambda^* \sim (aR_i)^{1/2}$, beyond which the pinning potential is irrelevant. If $L^* < \xi$, *the surface is basically free*. The crossover $L^* \sim \xi$ is exactly the condition (35). (In much the same way as a finite slope yielded a new characteristic length $d = n_s^{-1}$, an over-pressure introduces the length $(aR_i)^{1/2}$, which must be compared to ξ).

4. Growing interface under an applied force.

Instead of considering the *static* curvature of an interface under an applied force F, we assume that it moves while staying planar (on the average). We first consider an interface parallel to the crystal planes ($\theta = 0$), with a normal velocity u. We define a *mobility* $1/\eta$ as

$$u = F/\eta$$

η depends on T and possibly on F in the *non linear* nucleation regime. We want to understand that behaviour starting from the opposite ends of low and high temperatures.

4.1 $T \ll T_R$: HOMOGENEOUS NUCLEATION REGIME
[6]. — The free energy of a circular terrace with radius r on a flat facet (more exactly, it is a free enthalpy) is

$E(r) = 2 \pi r \beta - \pi r^2 Fa$. A critical germ has a radius r_c and energy E_c given by

$$r_c = \beta/Fa , \quad E_c = \pi \beta^2/Fa .$$

Such a germ only makes sense if $r_c \gg \xi$ (which implies $E_c \gg \beta \xi \sim T$). Thus, we have a choice of two regimes :

(i) $r_c \lesssim \xi$, $E_c \lesssim T$: there is no real nucleation. Thermal fluctuations on the flat facet are sufficient to provide growth, through a local attachment process controlled by a suitably renormalized friction η. The growth law is *linear* or quasi linear (η is nearly independent of F), characteristic of a *rough* interface for which the pinning potential is irrelevant.

(ii) $r_c \gg \xi$, $E_c \gg T$: then homogeneous nucleation controls growth (we discard possible Frank-Read sources).

We briefly recall [7] the main features of the non linear nucleation regime : an interface area S contains S/r_c^2 possible independent germs, each of which appears with a probability

$$1/\tau = 1/\tau_0 \exp(- E_c/T)$$

(the prefacor τ_0 requires a refined analysis). After a time t, the number of germs is $(S/r_c^2)(t/\tau)$: their *distance* is

$$\delta \sim r_c(\tau/t)^{1/2} .$$

Each germ grows radially with a velocity $v_s = \mu_s Fa$, where μ_s is the step *mobility*. The germs *coalesce* when their radius $r = v_s t$ is equal to δ, i.e. when

$$t = \bar{t} = [r_c^2 \tau/v_s^2]^{1/3} , \quad r = \delta = v_s \bar{t} = (v_s r_c^2 \tau)^{1/3} .$$

At any given time, the surface is *covered by growing germs*, with a size $\sim \delta$. The net vertical growth rate is

$$u = a/t \sim a(\mu_s^2/\beta^2 \tau_0)^{1/3}(Fa)^{4/3} \times$$
$$\times \exp(- \pi\beta^2/3 \, FaT) \quad (36)$$

(note the factor 1/3 in the Arrhenius factor). The growth law is highly non linear and u quickly vanishes as β becomes sizeable.

The crossover between regimes (i) and (ii) corresponds to $r_c = \xi$, which is nothing but (35). At a given $T < T_R$, F^* thus marks both the disappearance of a well defined facet in a steady equilibrium curved interface, and the transition nucleation $\leftrightarrow$ rough growth of a moving planar interface. Both in the static and in the dynamic problem, the transition is smooth : there is no sharp roughening transition when $F \neq 0$.

4.2 $T \gtrsim T_R$: RENORMALIZATION OF η. — The rough growth regime may then be treated within our scaling approach. Let u be the average normal velocity. The interface sees crystal planes drift by with a period $\tau = a/u$: the problem thus has another *unit of time* τ,

in much the same way as a tilted vicinal interface had a new unit of length $d = n_s^{-1}$. Our approach will be similar to that of section 3 : we shall *stop renormalization* when the relevant time scale is of order τ (the drifting of lattice planes then averages V to zero). We shall thus obtain an estimate of γ and η as a function of T and of F (*via* τ), thereby displaying the *onset of non linearities* and the smooth transition at $r_c \sim \xi$.

In the frame of the interface, the periodic potential is

$$- V \cos (2 \pi (z - ut)/a) .$$

Following the same course as in section 3, we construct scaling equations for γ and η which are similar to (21), except for an additional factor K_t resulting from the time lag in second order terms

$$K_t = \cos (2 \pi (t - t')/\tau) = \cos (2 \pi (\eta \rho^2 x/\gamma \tau))$$

(the reduced variable $x = \gamma(t - t')/\eta \rho^2$ is the same as in section 2). At a given stage of renormalization, the relevant length scale is $\rho \sim \bar{\Lambda}^{-1}$ (i.e. $\tilde{r} \sim 1$). The integral is dominated by $x \sim 1$, and thus the corresponding time scale is

$$t - t' \sim (\eta \rho^2/\gamma) \sim (\eta/\gamma \Lambda^2)$$

(it is the *diffusive* scale associated to ρ). K_t cuts off when this diffusive scale is $\sim \tau$, i.e. when

$$1/\Lambda \sim L^* = (\gamma \tau/\eta)^{1/2} = (\gamma a/F)^{1/2} . \quad (37)$$

(The mobility η disappears from (37), due to the lack of an intrinsic time unit in the problem). L^* marks the transition between two regimes :

(i) $\Lambda L^* \gg 1$: the motion of the interface has no noticeable effect on the scaling process, which proceeds as if the force F were zero.

(ii) $\Lambda L^* \ll 1$: K_t averages to zero and the renormalization of γ and η stops.

The scale L^* obtained in this *dynamical* argument is identical to the scale $(aR_i)^{1/2}$ derived from the bulge of a static interface : in either case, an applied force F stops renormalization when $\Lambda L^* \sim 1$ (thereby blurring the transition).

In principle, one may solve the exact equations (21) with the additional kernel K_t. A simpler qualitative picture is obtained by carrying the renormalization as if F were zero *up to the maximum scale* $\Lambda = 1/L^*$: experiments were interpreted in that way [9-10]. Such an approach makes sense if $L^* \ll \xi$, i.e. if the force F *exceeds* the characteristic F^* defined in (35) : the scaling theory is complementary to the nucleation regime.

In practice, the facet grows *as it were rough*. Since η *increases* as scaling proceeds, the macroscopic mobility $1/\eta$ decreases as temperature goes down. For an infinitesimal force F, it goes to the value calculated in section 2 when $T = T_R$ (with an infinite slope) ; below T_R, the mobility vanishes. When the force F is finite,

scaling stops earlier and $1/\eta$ is *larger,* resulting in a *non linearity* [1] which persists down to $F = 0$. Below T_R, it holds only when $F > F^*$. This behaviour is sketched in figure 6. Detailed calculations will be done in connection with experiments [9-10] : here we only note that $1/\eta$ is an increasing function of both T and F, which can be calculated explicitly within our « stopped renormalization scheme ».
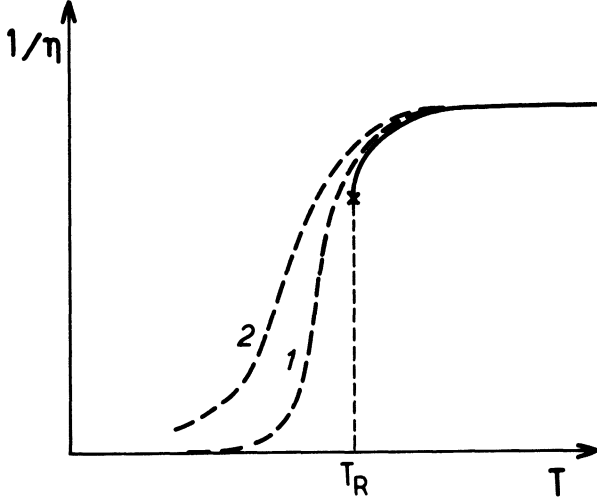

Fig. 6. — The mobility of a flat facet $1/\eta$ as a function of temperature for varying applied forces F. The full curve corresponds to $F \to 0$ (the facet does not grow below T_R). The dashed curves (1), (2) correspond to increasing forces : the transition between linear growth and nucleation is smooth at a temperature $T < T_R$.

When $L^* \gg \xi$, the scaling approach breaks down. Steps develop on the surface and facetting sets up. The renormalized periodic potential saturates to a value

$$V_{min} \sim T/\xi^2 \sim \gamma a^2/\xi^2 .$$

It is easily verified that $(2 \pi/a) V_{min} > F$: in the absence of fluctuations, the interface cannot slip over the maxima of V. It is indeed *pinned,* and the crystal grows by nucleation. It is gratifying that the crossover criterion is the same when approached from either side

$$F \sim \gamma a/\xi^2 \leftrightarrow \xi^2 \sim aR_i \leftrightarrow \xi \sim r_c .$$

However, we are lacking a theoretical description of the intermediate region.

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[1] Non linear crystal growth has been discussed by Saito [12], in a simple variational language, and by Neudecker [13] in a more elaborated renormalization approach. The resulting equation of motion is local in time, which we believe is incorrect once the cut off length scale L^* is exceeded. As a result, oscillatory growth is probably an artefact which is washed out by fluctuations on a macroscopic scale.

4.3 GROWTH OF A VICINAL INTERFACE. — Consider an interface tilted by a small angle θ, subject to a force F. Can we calculate $\gamma(F, \theta)$ and $\eta(F, \theta)$? We first consider the limit of *small F,* in which case the F dependence can be neglected. We already discussed the behaviour of γ (Fig. 5) : we now turn to η. The scaling approach predicts a slow decrease of $1/\eta$ as θ goes down : what we want to understand is the subsequent crossover when $\theta \sim a/\xi$.

For small F, nucleation is negligible. In the vicinal limit, $\theta \ll a/\xi$, growth occurs through the *sideways motion of vicinal steps.* Each step moves at a velocity $v_s = \mu_s Fa$, and the interface grows at a rate $u = n_s av_s$ — hence a *net* mobility

$$1/\eta = n_s a^2 \mu_s = \theta a \mu_s . \qquad (38)$$

(The linear dependence in θ is characteristic of the step regime.) In order to estimate μ_s, we start from the equation of motion of the profile $z(x, t)$ of an interface presenting a single step :

$$\eta_0(\partial z/\partial t) = - \eta_0 v_s(\partial z/\partial x) =$$
$$= \gamma \nabla^2 z - (2 \pi V/a)\sin (2 \pi z/a) + F \qquad (39)$$

(η_0, γ and V are suitably renormalized by short wave length fluctuations of scale $\ll \xi$; η_0 would be the actual mobility on that scale if the interface were not pinned by the periodic potential). In equilibrium ($F = 0$), the properties of a single step are easily obtained from (39) : its profile $z_0(x)$ and energy β are

$$z_0(x) = (2 a/\pi) \text{ Arctan } (\exp(x/\xi))$$

$$\beta = (4 a/\pi)(\gamma V)^{1/2}$$

$$\text{with} \quad \xi = (a/2 \pi)(\gamma/V)^{1/2} \sim (\gamma a^2/\beta) .$$

When $F \neq 0$, we multiply (39) by $\partial z/\partial x$ and we integrate from $(- \infty)$ to $(+ \infty)$: we thus obtain the condition

$$\eta_0 V_s \int_{-\infty}^{+\infty} (\partial z/\partial x)^2 dx = Fa$$

(which is nothing but *energy conservation*). In the linear regime, we can replace z by z_0, and thus

$$\mu_s = (\gamma/\eta_0 \beta) = (\pi^2 \xi/2 \eta_0 a^2)$$

μ_s is proportional to ξ (the force F acts on an « active » region of width ξ). Carrying μ_s into (38), we obtain the *macroscopic mobility*

$$1/\eta = \theta \gamma a/\beta \eta_0 \sim \theta \xi/a \eta_0 . \qquad (40)$$

The « step drift » regime and the « rough » regime join smoothly at $\theta \sim \xi/a$. The behaviour of $1/\eta(\theta)$ is sketched in figure 7 : after a slow initial drop in the scaling region, $1/\eta$ plunges down to zero when $\theta < \xi/a$.
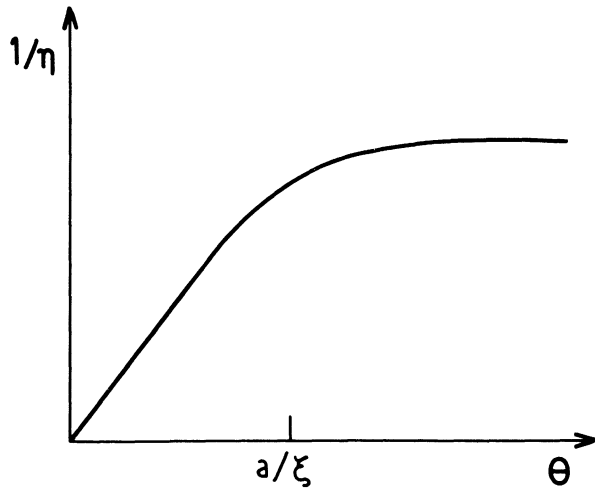
Fig. 7. — Sketch of the facet mobility $1/\eta$ at a fixed temperature $T < T_R$ as a function of the tilt angle θ. Note the smooth transition from a step regime at small θ to a rough surface at large θ.

When the force F is large, another question arises : we must compare the characteristic lengths due to the tilt, $d_1 \sim a/\theta$, and due to the growth rate, $d_2 = (\gamma a/F)^{1/2}$: thus a characteristic angle appears, $\theta_c = (Fa/\gamma)^{1/2}$. If either d_1 or d_2 is $\ll \xi$, the interface is rough.

(i) If $\theta > \theta_c$ (i.e. $d_1 < d_2$), the spatial cut off dominates. The growth law is strictly linear, with a weak angle dependence.

(ii) If $\theta < \theta_c$ (i.e. $d_1 > d_2$), the time cut off dominates. The mobility is θ-independent, but slightly non linear in F.

We can also calculate the surface energy α and the stresses $\gamma_\perp$, $\gamma_\parallel$. When $\theta \ll \theta_c$, α becomes analytic in θ and thus $\gamma_\parallel = \gamma_\perp$, as shown in figure 8.

Finally, for small forces F again, an interesting question is the crossover between step sideways drift and homogeneous terrace nucleation for very small
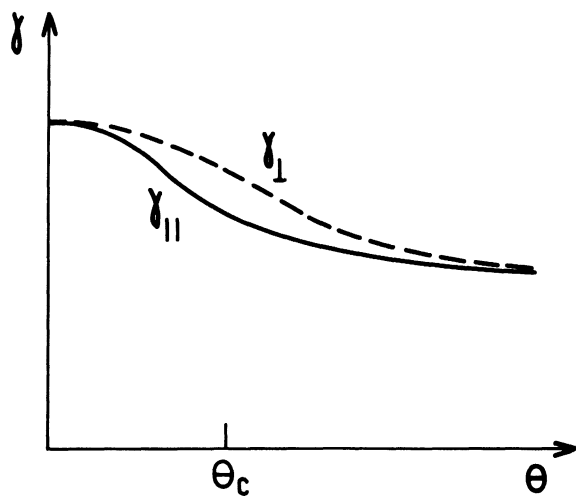
Fig. 8. — Sketch of the surface stiffness as a function of angle under a finite applied force $F > F^*$ (see (35)).

angles θ. The distance of vicinal steps is $d = a/\theta$, while the distance between nucleation terraces is δ : the relevant parameter is d/δ.

(i) If $\theta \gg a/\delta$, the vicinal step structure is hardly modified by a few, large nucleation terraces : the mobility (40) is controlled by sideways drift of vicinal steps.

(ii) If $\theta \ll a/\delta$, nucleation terraces are hardly affected by a few vicinal steps $(d \gg \delta)$: growth is dominated by nucleation. All physical quantities (mobility η, energy α, stiffness γ) are regular when $\theta \to 0$. In terms of the vicinal step density $n_s = a/\theta$, a reasonable interpolation for the surface energy seems to be

$$\alpha - \alpha_0 = (\beta/\delta)((1 + n^2 \delta^2)^{1/2} - 1)$$

which implies a saturation of the stiffness γ when $\theta \to 0$:

$$\gamma_\parallel = \gamma_\perp \sim (\beta \delta/a^2).$$

As a result, a growing facet is not strictly flat : it has a small curvature

$$(1/R_F) = (Fa^2/\beta \delta)$$

which grows rapidly as F increases (the tilt angle is $\theta \sim a/\delta$, corresponding to a facet radius $\sim R_F$ $\theta \sim \beta/Fa$, as expected). When F reaches the threshold F^*, the curvature is so large that the facet has practically disappeared : we enter the rough regime, with linear growth and no facetting. Even if it is small, such a curvature of a growing facet (due to rearrangement of the nucleation terraces) is essential in order to understand the smooth transition between facetted and rough states.

5. Conclusion.

In this paper, we tried to give a comprehensive review of both static and dynamic aspects of the roughening transition. Following reference [5], we gave a formulation of the scaling process which is exempt from the usual pitfalls. We examined the relationship between the static and dynamic methods (which are only identical at the fixed point). Our detailed analysis provides an explicit form of the renormalization constants for the surface stress γ and friction η : our results differ appreciably from those of Chui and Weeks [6], who probably relied on a « logarithmic » approximation, valid only at the transition $T = T_R$. These more precise results are used elsewhere in interpreting experiments [9-10].

Finally, we analysed the various crossovers between the fixed flat interface and other more complicated situations, such as

(i) Static vicinal surfaces, with a finite tilt θ.
(ii) Growing facet with a finite velocity u.
(iii) Growing vicinal surfaces.

In each case, we approached the crossover from both ends. On the « rough » side, we used a stopped

renormalization description, the cut off being either spatial (for a tilt θ) or temporal (for a velocity u). In this way, we explain the small angle dependence of γ or the small non linearity of growth. In the opposite end, we use a *step picture*, based on the interaction of vicinal steps or on nucleation of two dimensional terraces. These two limits join smoothly, but the intermediate region lies out of the range of our theory. It can be described only in exactly soluble models, such as the 6-vertex model of Van Beijeren [3].

One feature emerges from this analysis : the roughening transition is sharp only for *a flat, infinite interface at rest*. If the interface is tilted, the transition is blurred when crystal steps begin overlapping. A similar blurring occurs if we apply a *finite overpressure force F*, both in the static case (bent interface with a finite facet radius),

or in the dynamic regime (growing interface). In all these examples, a gradual crossover occurs when the correlations length $\xi(T)$ is comparable to some new characteristic length (step distance $d = a/\theta$ for a vicinal surface, critical nucleation radius $r_c = \beta/F$). As a result, the blurred transition occurs *below T_R* : the *rough behaviour extends below the nominal transition temperature*. Such an analysis is essential in fitting experimental result : this comparison will be done in another paper.

Acknowledgments.

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