

A Relaxed Model for Step-Terraces on Crystalline Surfaces

Matthias Kurzke*

University of Leipzig, Germany
kurzke@mathematik.uni-leipzig.de

Marc Oliver Rieger†

Scuola Normale Superiore, Piazza dei Cavalieri, 7, 56126 Pisa, Italy
rieger@sns.it

Received October 28, 2002

We study a variational problem that has been introduced to describe step-terraces on surfaces of so-called “unorthodox” crystals. Motivated by physical considerations, we use Γ -convergence to derive a simplified model that can be solved explicitly.

Keywords: Surfaces of crystals, step-terraces, unorthodox crystals, variational problems, Gamma-convergence

1991 Mathematics Subject Classification: 49, 74

1. Introduction

For the understanding of crystalline growth processes, the form of step-terraces on the crystalline surface plays an important role (see e.g. [5]). The edges of these steps usually form oscillations in space that become larger when the equilibrium temperature rises. This behaviour is called “orthodox” and had been explained by Herring, Mullins and others (see e.g. [7]) by thermodynamical effects. However, recently crystals have been studied which are “unorthodox” in the sense that lower temperatures lead to larger oscillations and the step profile takes a saw-tooth structure for low temperatures (Fig. 1.1a) and not a straight line (Fig. 1.1b) as the classical theory would predict [3]. To describe this situation, a refined model has been suggested by Hannon, Marcus and Mizel [4]. To state it we first need some definitions:

Let $\theta \in W^{1,2}((0, S), [-\frac{\pi}{2}, +\frac{\pi}{2}])$ describe the angle of the step profile relative to a straight line profile. Let $\beta \in C^1[-\frac{\pi}{2}, +\frac{\pi}{2}]$ with $\min \beta = \beta(\frac{\pi}{2}) = \beta_0 > 0$ and $\beta(\alpha) = \beta(-\alpha)$ for all $\alpha \in [-\frac{\pi}{2}, +\frac{\pi}{2}]$. Define

$$X(s) := \int_0^s \cos \theta(\tau) d\tau, \quad (1)$$

$$Y(s) := y_0 + \int_0^s \sin \theta(\tau) d\tau, \quad (2)$$

*Supported by the DFG Graduiertenkolleg “Analysis, Geometrie und ihre Verbindung zu den Naturwissenschaften”

†Supported by the Center for Nonlinear Analysis under NSF Grant DMS-9803791.

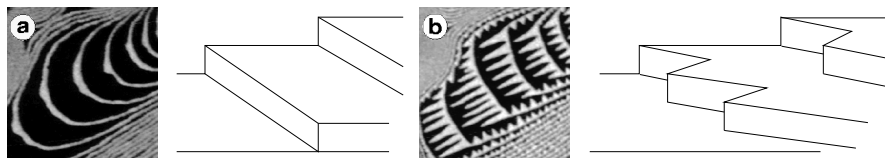


Figure 1.1: Experimental pictures [3] and schematic sketches of step terraces on the surface of an unorthodox crystal for high (a) and low (b) temperatures.

and let L , ρ and σ be positive constants. Minimize the energy

$$E(\theta) := \int_0^S \rho |\theta'|^2 + \beta(\theta) + \sigma Y^2 ds, \quad (3)$$

subject to the constraints

$$\int_0^S \cos \theta(\tau) d\tau = L, \quad \int_0^S \sin \theta(\tau) d\tau = 0, \quad (4)$$

in $S \geq L$ and θ . The step profile can be described by the graph $(X(s), Y(s))_{s \in [0, S]}$. The first constraint in (4) expresses that the profile has to extend to $(0, L)$ in the x -direction, while the second constraint ensures the boundary condition $Y(0) = Y(S)$ (compare Fig. 1.2).

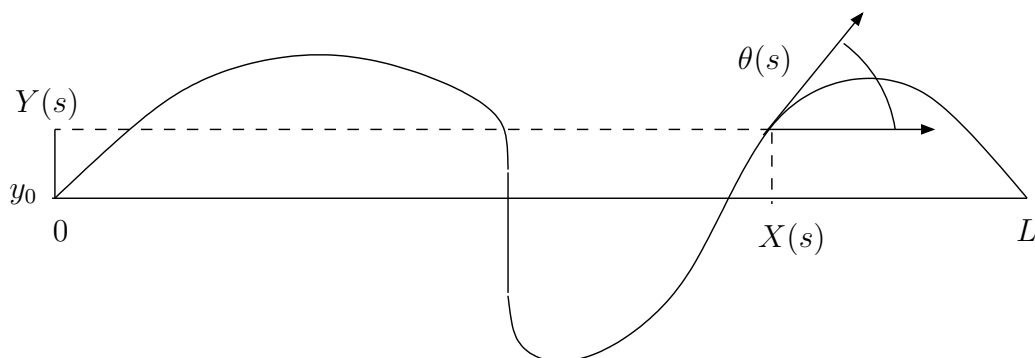


Figure 1.2: The graph of a typical function θ .

The energy (3) consists of three parts, the last two are physically well motivated, whereas the first one has purely a technical reason: Without this term the problem would not admit a minimizer in a classical sense [4].

The minimization problem (3)–(4) admits a solution as has been shown in [4]. However there are still difficulties in calculating a solution that originate in the fact that Y cannot be written as a function of x , since the graph (X, Y) may have vertical parts, and in the unusual side constraints.

Our attempt was to consider a certain Γ -limit of this problem. This gives us a simplified energy functional that can be easily minimized and that reflects the relevant physical features of the problem. Additionally the solutions of this relaxed problem may give some insight into the solutions of the original problem.

In the next section we reformulate the problem above to derive its Γ -limit. In Section 3 we will calculate explicit solutions for the limit problem.

2. The Γ -limit

First we need the notion of piecewise Sobolev functions as given in the following straightforward definition:

Definition 2.1 (Piecewise Sobolev functions). Let $q \geq 1$. Let Δ_k be the set of all strictly increasing $(x_i)_{i=0,\dots,k}$ with $x_0 = 0$ and $x_k = L$. A function $u \in L^1(0, L)$ is a *piecewise Sobolev function* $W_p^{1,q}(0, L)$ if there exists $k \in \mathbb{N}$ and $(x_i) \in \Delta_k$, such that $u|_{(x_i, x_{i+1})} \in W^{1,q}(x_i, x_{i+1})$ for $i = 0, \dots, k - 1$.

We say that a sequence $(u_n) \subset W_p^{1,q}(0, L)$ converges to a function $u \in W_p^{1,q}(0, L)$ whenever $\|u_n - u\|_\infty \rightarrow 0$ and

$$\liminf_{n \rightarrow \infty} \inf_k \inf_{(x_i) \in \Delta_k} \left\{ \sum_{i=0}^{k-1} \|u_n - u\|_{W^{1,q}(x_i, x_{i+1})} \right\} = 0.$$

(Here we define $\|v\|_{W^{1,q}} := \infty$ for all $v \notin W^{1,q}$.)

Reformulation of the problem

We want to derive an expression corresponding to (3) for $W_p^{1,q}$ functions depending on X rather than on s . First we consider subintervals $J \subset [0, L]$ where the $(X(s), Y(s))$ corresponding to $\theta(s)$ has no vertical parts and is hence a classical graph $y(x)$. With $y = Y(s)$, $x = X(s)$ and hence $y(x) = Y(X^{-1}(s))$ we calculate (denoting $\dot{\cdot} = \frac{d}{ds}$, $' = \frac{d}{dx}$):

$$y'(x) = \frac{\dot{Y}}{\dot{X}}(X^{-1}(x)) = \tan \theta(X^{-1}(x))$$

and

$$y''(x) = (1 + \tan^2 \theta) \dot{\theta}(X^{-1}(x)) \frac{1}{\dot{X}(X^{-1}(x))} = \frac{1 + \tan^2 \theta}{\cos \theta} \dot{\theta} = \pm (1 + \tan^2 \theta)^{3/2} \dot{\theta}.$$

With the line element ds transforming like

$$ds = \sqrt{1 + |y'|^2} dx,$$

we obtain the expression for the energy contribution in J as

$$\int_J \left(\rho \frac{y''^2}{(1 + y'^2)^3} + \beta(\arctan y') + \sigma y^2 \right) \sqrt{1 + |y'|^2} dx.$$

On the vertical parts we have $\dot{\theta} = 0$ hence we get the energy contribution simply as

$$\int_{s_1}^{s_2} \beta(\pm \frac{\pi}{2}) + \sigma Y^2(s) ds.$$

For $Y(s_1) = y(x_-)$ and $Y(s_2) = y(x_+)$, $y_1 = \min(y(x_-), y(x_+))$, $y_2 = \max(y(x_-), y(x_+))$ we can write this (using arc-length parametrization) as

$$\int_{y_1}^{y_2} \beta_0 + \sigma t^2 dt = \beta_0(y_2 - y_1) + \frac{\sigma}{3}(y_2^3 - y_1^3),$$

so the contribution of a jump at x is

$$\beta_0|y(x+) - y(x-)| + \frac{\sigma}{3}|y(x+)^3 - y(x-)^3|.$$

Collecting all terms, we arrive at the new energy functional given by

$$\begin{aligned} E(y) &= \sum_i \int_{J_i} \left(\rho \frac{y''^2}{(1+y'^2)^3} + \beta(\arctan y') + \sigma y^2 \right) \sqrt{1+|y'|^2} dx \\ &+ \sum_{\text{jumps}} \beta_0|y(x+) - y(x-)| + \frac{\sigma}{3}|y(x+)^3 - y(x-)^3|. \end{aligned} \quad (5)$$

Renormalization and statement of Γ -limit

In order to derive a Γ -limit, we assume that ρ and σ have the following scaling property with respect to an additional parameter ε :

$$\rho = \rho_0 \varepsilon^2, \quad \sigma = \sigma_0 \varepsilon.$$

Then we can determine the asymptotic behaviour of $\frac{1}{\varepsilon} E_\varepsilon$ as $\varepsilon \rightarrow 0$. Since $\inf \left(\beta(\arctan y') \sqrt{1+y'^2} \right) > 0$, we have to renormalize the energy by subtracting this infimum, so we define

$$B(z) := \beta(\arctan z) \sqrt{1+z^2} - \inf_{z \in \mathbb{R}} \left(\beta(\arctan z) \sqrt{1+z^2} \right), \quad (6)$$

and get the new functional

$$\begin{aligned} H_\varepsilon(y) &:= \sum_i \int_{J_i} \left(\varepsilon \rho_0 \frac{y''^2}{(1+y'^2)^3} + \sigma y^2 \right) \sqrt{1+|y'|^2} + \frac{1}{\varepsilon} B(y') \, dx \\ &+ \sum_{\text{jumps}} \frac{1}{\varepsilon} \beta_0|y(x+) - y(x-)| + \frac{\sigma}{3}|y(x+)^3 - y(x-)^3| \end{aligned} \quad (7)$$

To simplify our exposition, we will only treat the (generic) case where $B^{-1}(0) = \{\pm\alpha\}$ for some $\alpha > 0$.

In the following we denote the discontinuity set of a function v by S_v and the number of points in a set X by $\mathcal{H}^0(X)$. Then we can formulate the following result for the limit of the functionals H_ε :

Theorem 2.2 (Γ -limit). *For $\varepsilon \rightarrow 0$ the functionals H_ε Γ -converge in the $W_p^{1,1} \cap L^\infty$ topology to*

$$H(y) = \begin{cases} \sigma \sqrt{1+\alpha^2} \int_0^L y^2 dx + K \mathcal{H}^0(S_{y'}) & \text{if } y \in W^{1,1}(0, L) \text{ and} \\ & y' \in BV([0, L], \{\pm\alpha\}), \\ +\infty & \text{else,} \end{cases} \quad (8)$$

where K is given by

$$K := \sqrt{\rho_0} K_0 \quad (9)$$

$$:= 2\sqrt{\rho_0} \int_{-\alpha}^{\alpha} \frac{B(t)^{1/2}}{(1+t^2)^{5/4}} dt \quad (10)$$

and S_u denotes the jump set of a BV function u .

We observe that the term of (7) which accounts for the energy of jumps in y vanishes in the limit. The reason for this is simply that a jump in y corresponds to an infinite derivative of y , and hence an infinite limit energy.

Proof of the Theorem.

We first consider the functional for the highest order terms:

$$F_\varepsilon(y) := \int_I \varepsilon \rho_0 \frac{|y''|^2}{(1 + |y'|^2)^{5/2}} + \frac{1}{\varepsilon} B(y') dx, \tag{11}$$

for all $y \in \mathcal{A}$ where

$$\mathcal{A} := \left\{ y \in W_p^{1,2}(0, L), \frac{|y''|^2}{(1 + |y'|^2)^{5/2}} \in L^1(0, L), y(0) = y(L) = y_0 \right\}.$$

If the first term was just $\varepsilon \rho_0 |y''|^2$, then (11) would describe a standard Modica-Mortola functional (see [6] or [2]). But the more complicated problem can still be treated with the same methods, following the ideas of Alberti [1]. The only difference is that due to the lack of an adequate growth condition on B , we cannot prove compactness, i.e. equicoercivity. However, we can still prove Γ -convergence to the limit functional

$$F(y) := \begin{cases} K \mathcal{H}^0(S_{y'}) & \text{if } y \in W^{1,1}(0, L) \text{ and } y' \in BV(I, \{\pm\alpha\}) \\ +\infty & \text{else.} \end{cases} \tag{12}$$

Lemma 2.3 (Lower bound inequality). *Let $y_\varepsilon \rightarrow y$ in the strong $W^{1,1}$ topology. Then $F(y) \leq \liminf_{\varepsilon \rightarrow 0} F_\varepsilon(y_\varepsilon)$.*

Proof. We can assume w.l.o.g. that $F_\varepsilon(y_\varepsilon) \leq M < \infty$. Using the inequality $\varepsilon a^2 + \frac{1}{\varepsilon} b^2 \geq 2ab$ we calculate

$$F_\varepsilon(y_\varepsilon) \geq 2\sqrt{\rho_0} \int_I \frac{B(y')^{1/2}}{(1 + |y'|^2)^{5/4}} |y''| dx. \tag{13}$$

Setting $h(t) := 2\sqrt{\rho_0} \frac{B(t)^{1/2}}{(1+t^2)^{5/4}}$ and $H(t) = \int_0^t h(s) ds$ and using the chain rule, (13) leads to

$$F_\varepsilon(y_\varepsilon) \geq \int_I h(y'_\varepsilon) |y''_\varepsilon| dx = \int_I \left| \frac{d}{dx} H(y'_\varepsilon) \right| dx = |H(y'_\varepsilon)|_{BV(I)}. \tag{14}$$

(There is no problem at the discontinuities of y_ε , since $\lim_{z \rightarrow \pm\infty} H(z) = 0$.)
As (at least for a subsequence) $H(y'_\varepsilon) \rightarrow H(y')$ in L^1 , the lower semicontinuity of the total variation yields

$$|H(y')|_{BV(I)} \leq \liminf_{\varepsilon \rightarrow 0} F_\varepsilon(y_\varepsilon). \tag{15}$$

From $B(y'_\varepsilon) \rightarrow B(y')$ in L^1 (for a subsequence) and $M \geq \frac{1}{\varepsilon} \int_I B(y'_\varepsilon) dx$ we deduce $\int_I B(y') dx = 0$ and thus $y' \in \{\pm\alpha\}$ a.e. in I . This implies $H(y') \in \{H(\pm\alpha)\}$ a.e., so the total variation of $H(y')$ is given by the number of jumps of y' multiplied with $|H(\alpha) - H(-\alpha)| = K$. □

Before we prove the upper bound inequality, we note that F_ε really depends only on the derivative of y , apart from the boundary condition. We thus set

$$G_\varepsilon(u, J) := \int_J \varepsilon \rho_0 \frac{|u'|^2}{(1 + u^2)^{5/2}} + \frac{1}{\varepsilon} B(u) dx, \tag{16}$$

a functional that also depends (as a positive measure) on the integration domain and has (if we define $u_\varepsilon(x) = u(\varepsilon x)$) the scaling property

$$G_\varepsilon(u, \varepsilon J) = G_1(u_\varepsilon, J). \tag{17}$$

This scaling helps us to determine the optimal profile.

Lemma 2.4 (The optimal profile problem).

$$\inf\{G_1(u, \mathbb{R}) : u \in C^1(\mathbb{R}, [-\alpha, \alpha]), \lim_{x \rightarrow -\infty} u(x) = -\alpha, \lim_{x \rightarrow \infty} u(x) = \alpha\}$$

is attained at a function γ and is equal to K . We can choose γ such that $\gamma(x) = -\gamma(-x)$.

Proof. This follows in the same way as in Proposition 2 of [1]. The symmetry of γ follows easily from the symmetry of B . □

Lemma 2.5 (The upper bound). *Let y be a function with $F(y) < \infty$. Then there is a sequence $y_\varepsilon \rightarrow y$ in $W^{1,1}$ with $\lim_{\varepsilon \rightarrow 0} F_\varepsilon(y_\varepsilon) = F(y)$.*

Proof. As $F(y) < \infty$, y is a saw-tooth function with slopes $\pm\alpha$. We choose a $\delta > 0$ such that $3\delta < \min\{|a - b| : a \neq b \in S_{y'}\}$ and define y_ε as y outside $B_{\delta+\varepsilon}(S_{y'})$ (see Fig. 2.1).

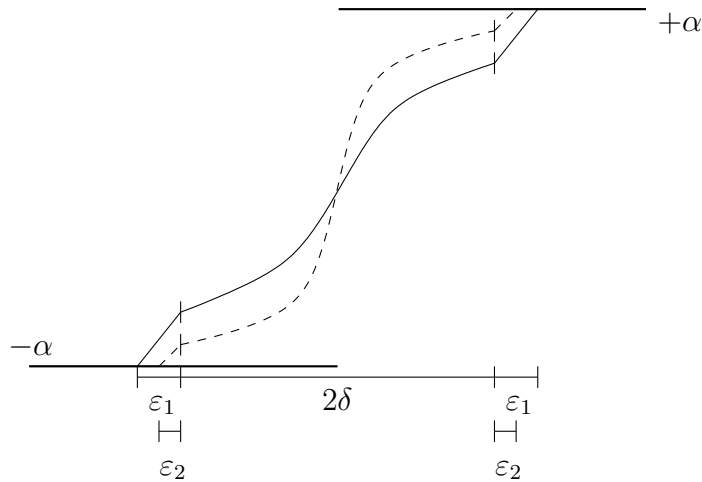


Figure 2.1: The function y' (thick line) and two approximating functions where δ is fixed, but ε takes the values ε_1 (simple line) and ε_2 (dotted line). For $\varepsilon \rightarrow 0$ the approximations converge to y' .

Let $x_0 \in S_{y'}$, w.l.o.g. $x_0 = 0$. Define $y_\varepsilon(x) := y(0) + \int_0^x \gamma(t/\varepsilon) dt + \eta_\varepsilon$ inside $B_\delta(0)$. On the remaining part, we define the function by linear interpolation of the derivative (and then

integrating), this also defines $\eta_\varepsilon \rightarrow 0$ which is to be chosen such that everything matches. Following [1], we finally get $y_\varepsilon \rightarrow y$ in $W_p^{1,1}$ and $F_\varepsilon(y_\varepsilon) \rightarrow F(y)$.

Lower order terms

Now we consider the lower order terms in the functional (7). We prove that they are continuous with respect to the $W_p^{1,1}$ -convergence, and hence can be handled as an independent perturbation of the functional while taking the Γ -limit.

We define

$$I_1(y) := \int_0^L \sigma y^2 \sqrt{1 + |y'|^2} dx, \tag{18}$$

and

$$I_2^\varepsilon(y) := \sum_{\text{jumps}} \left(\frac{1}{\varepsilon} \beta_0 |y(x-) - y(x+)| + \frac{\sigma}{3} |y(x+)^3 - y(x-)^3| \right). \tag{19}$$

Let $y_n \rightarrow y$ in $W_p^{1,1}$ with $F_\varepsilon(y_n)$ uniformly bounded in n . We show that this leads to $I_1(y_n) \rightarrow I_1(y)$ and $I_2^\varepsilon(y_n) \rightarrow I_2^\varepsilon(y)$.

For I_1 we can prove this by the following estimate:

$$\begin{aligned} I_1(y_n) - I_1(y) &= \sigma \int_0^L \left(y_n^2 \sqrt{1 + |y_n'|^2} - y^2 \sqrt{1 + |y'|^2} \right) dx \\ &\leq \|y_n^2 - y^2\|_\infty (1 + \|y_n'\|_{L^1}) \\ &\quad + \|y^2\|_\infty \int_0^L \left(\sqrt{1 + |y_n'|^2} - \sqrt{1 + |y'|^2} \right) dx \\ &\leq \underbrace{\|y_n^2 - y^2\|_\infty}_{\rightarrow 0} \underbrace{(1 + \|y_n'\|_{L^1})}_{\text{bounded}} + \underbrace{\|y^2\|_\infty}_{\text{bounded}} \underbrace{\|y_n' - y'\|_{L^1}}_{\rightarrow 0}. \end{aligned}$$

For I_2^ε it follows from the convergence of y_n in the L^∞ -norm ensuring that

$$|y_n(x-) - y_n(x+)| - |y(x-) - y(x+)| \rightarrow 0.$$

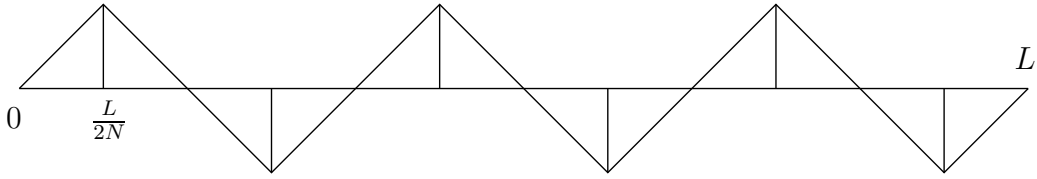
We can now add the limit terms to F and get the Γ -limit of the complete functional. This proves the theorem. □

3. Explicit solutions

Let $\tilde{\sigma} := \sigma \sqrt{1 + \alpha^2}$ and $\tilde{\rho} := K$. Then we can write the limit problem in the generic case as follows:

$$\text{Minimize } E(y) := \int_0^L \tilde{\sigma} y^2 + \tilde{\rho} \mathcal{H}_0(S_{y'}) , \tag{20}$$

for $y \in H^1(0, L)$ subject to the side constraints $y(0) = y(L) = 0$ and $|y'| = \alpha > 0$ a.e. Let y be a minimizer of (20). We assume that y' has $N \in \mathbb{N}$ jumps $(x_i)_{i=1, \dots, N}$. By applying Jensen's inequality we see that $x_i = L(i - 1/2)/N$. For a given N this gives an

Figure 3.1: The function y for $N = 6$ and $\alpha = 1$

implicit formula for y (up to the sign), see Fig. 3.1.

We calculate its energy E_N as follows:

$$\begin{aligned} E_N &= 2N \int_0^{L/2N} \tilde{\sigma} \alpha^2 x^2 dx + \tilde{\rho} N \\ &= \tilde{\sigma} \alpha^2 \frac{L^3}{4N^2} + \tilde{\rho} N. \end{aligned}$$

To compute the optimal N , we take the derivative of E_N with respect to N .

$$\frac{d}{dN} E_N = \tilde{\rho} - \tilde{\sigma} \alpha^2 \frac{L^3}{2N^3}.$$

This becomes zero if

$$N_0 = 2^{-1/3} \alpha^{2/3} L \sqrt[3]{\frac{\tilde{\sigma}}{\tilde{\rho}}}. \quad (21)$$

Since $\lim_{N \rightarrow 0} E_N = \lim_{N \rightarrow +\infty} E_N = +\infty$, we see that E_N is minimal at N_0 . – More precisely we need $N \in \mathbb{N}$, so the N we are looking for is one of the two natural numbers closest to N_0 .

This completely characterizes the minimizer. The saw-tooth structure of the result is in good correspondence with the physical experiments (see Fig. 1.1). The optimal number of oscillations depends only on α and on the quotient of $\tilde{\sigma}$ and $\tilde{\rho}$ (which itself depends on β). This is consistent with the underlying physics.

If we take into account the definition of K and that (for sufficiently large slopes α) we have $\sqrt{1 + \alpha^2} \approx \alpha$, then we get the simplified formula

$$N_0 \approx 2^{-1/3} \alpha K_0^{-1/3} L \sigma^{1/3} \rho_0^{-1/6}.$$

Since K_0 is likely to increase with increasing α , this predicts that N_0 is growing slower than α (assuming that σ and ρ_0 do not change significantly). We can confirm this prediction by taking a closer look to experimental data obtained by Hannon et al.[3], where in an unorthodox crystal α and N_0 are both increasing with decreasing temperature, but α is growing much faster than N_0 . It would be interesting to verify this prediction in a more quantitative way or to perform physical experiments with different values for $\sigma^{1/3} \rho_0^{-1/6}$.

Acknowledgements. We are grateful to Victor Mizel for his help and for introducing the topic to us and to James B. Hannon for providing us with his experimental data. The main results were obtained during a stay of the second author at the Max Planck Institute for Mathematics in the Sciences in Leipzig, Germany, and he expresses his thanks for the hospitality.

References

- [1] G. Alberti: Variational models for phase transitions, an approach via γ -convergence, in: *Calculus of Variations and Partial Differential Equations, Topics on Geometrical Evolution Problems and Degree Theory*, G. Buttazzo et al. (ed.), Springer, Berlin (2000) 17–32.
- [2] G. Dal Maso: *An Introduction to Γ -Convergence*, Birkhäuser Boston, Boston, MA (1993).
- [3] J. Hannon et al.: Step faceting at the (001) surface of boron doped silicon, *Phys. Rev. Letter* 79 (1997) 4226–4229.
- [4] J. Hannon, M. Marcus, Victor J. Mizel: A variational problem modelling behavior of unorthodox silicon crystals, *ESAIM Control Optim. Calc. Var.* 9 (electronic) (2003) 145–149.
- [5] H. C. Jeong, E. D. Williams: Steps on surfaces: Experiment and theory, *Surface Science Reports* 34 (1999) 175–294.
- [6] L. Modica, S. Mortola: Il limite nella γ -convergenza di una famiglia di funzionali ellittici, *Boll. Un. Mat. Ital. A* (5) 14(3) (1977) 526–529.
- [7] W. W. Mullins: Theory of thermal grooving, *J. Appl. Physics* 28 (1957) 333–339.