

External field as a tool for measuring absolute values of step–step interaction

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Abstract

In absence of any external field, the equilibrium profile $z(x)$ of a vicinal rounded part tangentially joined to a flat facet is known to follow a universal scaling law $z(x) \propto x^{3/2}$. This universal behaviour is modified when the crystal is plunged in an external field. The deviation from the universal Gruber–Mullins–Pokrovsky–Talapov behaviour depends on the facet orientation, the chemical potential of the crystal and the external field. We show that measuring this deviation is enough to provide absolute value of the step–step interaction. Applications to gravitation and centrifugation fields are discussed.

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1. Introduction

The equilibrium shape of faceted crystals puzzled physicists for a long time. A first step towards an explanation of equilibrium crystal shapes has been done by Curie [1] then Wulff [2] who have shown that the equilibrium shape of a free crystal is the shape that minimises its total surface free energy under the constraint of constant volume. In the ground state ($T = 0$) theoretical crystal shapes are composed of facets separated by sharp edges whereas increasing the temperature the facets shrink in size and become connected by rounded parts. The local profile of the curved region near a singular facet depends on the exact analytical form of the surface energy of the vicinal surface connected to the singular facet [3,4]. More precisely a vicinal rounded part tangentially joined to a flat facet can be described by a

local scaling law $z(x) = ax^n$. The exponent $n = 3/2$ has been shown to be universal within a large class of models describing crystal surfaces, it is called the Gruber–Mullins–Pokrovsky–Talapov (GMPT) exponent [5,6]. Since the local equilibrium shape can be described as an equilibrium of steps, the coefficient a depends on two quantities: the step–step interaction and the chemical potential of the crystal.

In 1988, Avron et al. [7] showed, using a 2D model, that gravity transmutes the GMPT exponent from $3/2$ to 3 when moving away from the singular surface. Avron et al. [7] essentially studied the crossover between the $x^{3/2}$ profile close to the facet and the x^3 profile far from the facet but did not give the complete analytical expression of the profile $z(x)$ in presence of gravity. In this short paper we intend to obtain an exact expression of the local profile of a crystal plunged in a given external field that may be uniform or not. We will show that as soon as a crystal is plunged in an external field, the GMPT exponent $n = 3/2$ is no more valid [7]. Moreover the deviation we find provides the opportunity to extract independently the step–step interaction and the chemical potential.

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The paper is organised in three parts. The first section, devoted to the description of the local equilibrium shape in presence of an external field, completes the work of Avron et al. [7]. The second part concerns the use of an external field as a tool for measuring absolute values of the step–step interaction. Lastly in a short conclusion we discuss the main limitations of the method.

2. Equilibrium shape in presence of an external field

2.1. General considerations: Euler–Lagrange equation in presence of an external field

In a field-free environment, the equilibrium shape of a body is the shape that minimises its surface free energy $\int_S \gamma(\vec{n})dS$ at constant volume where $\gamma(\vec{n})$ is the anisotropic surface free energy, \vec{n} a unit vector normal to the surface S of the crystal and dS a surface element [1,2]. It results the Wulff theorem, which states that the equilibrium shape is the pedal of the surface free energy $\gamma(\vec{n})$ [2].

For a crystal plunged in an external field, the equilibrium shape is the one that minimises the total free energy (for a discussion see [7,8])

$$\int_S \gamma(\vec{n})dS + \int_V \Phi(\vec{r})dV \text{ at constant volume } V \quad (1)$$

Now the total energy contains $\Phi(\vec{r})$ the external field potential energy density. Obviously dV is a volume element.

For the sake of simplicity, we will only consider a two-dimensional (2D) case where the equilibrium shape is an

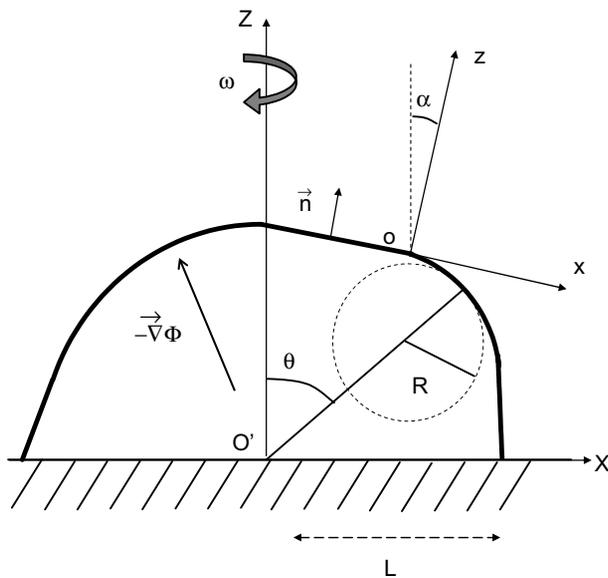


Fig. 1. Scheme of the 2D crystal under consideration. ($O'XZ$) and (OxZ), respectively, are the laboratory referential and the referential attached, to the facet edge (z is normal to the facet and makes an angle α with respect to ($O'Z$)). θ is the polar angular coordinate of the profile. $-\vec{\nabla}\Phi$ is the external field applied to the crystal. R is the local radius of curvature of the crystal and L is the characteristic size of the crystal. In case of crystal rotation ω is the angular velocity.

equilibrium contour. The geometrical configuration we will use is reported in Fig. 1: a crystal deposited on a foreign (but pseudomorphic or structureless) substrate¹ with a facet tangentially joined to a rounded part. We will note (OxZ) the local referential associated to a facet edge and ($O'XZ$) the laboratory referential.

For a rounded part, the surface energy is a continuous function of the local slope $p = \pm dz/dx$ so that the integral (1) to be minimised reads:

$$\int G(x, z, p)dx = \int [\gamma(p)\sqrt{1+p^2} - \lambda z + \int \Phi(x, \varsigma)d\varsigma + \gamma_{AB}]dx \quad (2)$$

The quantity $\beta(p) = \gamma(p)\sqrt{1+p^2}$ in Eq. (2) is the so-called “projected energy”, λ is a Lagrange multiplier (in fact the chemical potential change [10]) introduced because of the constraint of constant volume (here area, $\int z(x)dx$), $\int \Phi(x, \varsigma)d\varsigma$ is the potential energy density of the external field integrated on the z axis and γ_{AB} is the interfacial free energy.

The starting point for an analytic description of the local shape is the analytical expression of the orientation dependence of the surface free energy. For this purpose, using the Terrace-Ledge model [11], the “projected energy” is generally written:

$$\beta(p) = \beta_0 + \beta_1|p| + \beta_3|p|^3 \quad (3)$$

where β_0 is the surface free energy density of the flat terraces, β_1 the free energy density of an isolated step, β_3 the step–step interaction energy density² due to entropy, elastic or electrostatic repulsion (for a review see [12]) and p the local slope in the local referential $z(x)$ (see Fig. 1).

The function $G(x, z, p)$, which minimises (2) is solution of the Euler–Lagrange equation [13]:

$$\frac{\partial G}{\partial z} - \frac{d}{dx} \frac{\partial G}{\partial p} = 0 \quad (4)$$

Using the expression of $G(x, z, p)$ given in (2) with Eq. (3), the Euler–Lagrange equation reads:

$$\frac{\partial^2 z}{\partial x^2} \frac{\partial^2 \beta}{\partial p^2} = -\lambda + \Phi(x, z) \quad (5)$$

Introducing the local polar angle θ of the rounded part in the $Z(X)$ referential (see Fig. 1) as a new variable, Eq. (5) can also be written:

$$\tilde{\gamma}/R = -\lambda' \quad (5')$$

where R is the local radius of curvature of the profile (see Fig. 1). The quantity $\tilde{\gamma} = \gamma + \partial^2 \gamma / \partial \theta^2$ defines the so-called surface stiffness and $\lambda' = \lambda - \Phi(x, z)$ is a generalized chemical potential that contains the external field potential energy density $\Phi(x, z)$ as a correction to the usual chemical

¹ For non-pseudomorphic crystalline substrate, bulk and surface elasticity intervene (see for example [9]).

² Notice that in this model there is no p^2 term in the development of $\beta(p)$.

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