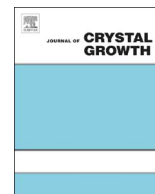




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Effect of the roughening transition on the vicinal surface in the step droplet zone

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ABSTRACT

For vicinal surfaces around the (001) surface inclined towards the $\langle 111 \rangle$ direction, the influence of roughening transitions on the surface tension and on step droplets is studied numerically. The surface tension is calculated using a restricted solid-on-solid model with a point-contact type step–step attraction (p-RSOS model) on a square lattice. To ensure the reliability of the calculations, the density matrix renormalization group method is used. The growth rate of the vicinal surface near equilibrium is also calculated by the Monte Carlo method. It is found that the roughening transition changes the morphology around the (001) surface, and the roughening transition affects the size of locally merged steps (step droplets).

1. Introduction

In 1963, Cabrera and Coleman [1] showed that if the surface free energy has a “type II” anomaly, the equilibrium shape of a crystal droplet (equilibrium crystal shape, ECS) has a first-order shape transition¹; moreover, the instability with respect to macrostep formation may result from the anomalous surface free energy at equilibrium.

There has long been a need for a means of calculating anisotropic surface tension using a microscopic model in order to better understand the morphology and rate of growth of such crystals. However, due to the low dimensionality of the surface and of steps, neither mean field calculations nor quasi-chemical approximations are reliable for calculating surface thermodynamic quantities [3].

In our previous work [4–7], we calculated the slope dependence of the surface tension using a restricted solid-on-solid (RSOS) model with a point-contact type step–step attraction (p-RSOS model). To obtain reliable results, we used the density matrix renormalization group (DMRG) method [8,9], which is known to be effective for one-dimensional quantum spin systems.

From the results on the slope dependence of the surface tension, we found that the surface tension is discontinuous at low temperatures for a vicinal surface inclined towards the $\langle 111 \rangle$ direction. The discontinuity of the surface tension leads to the formation of faceted macrosteps on a vicinal surface, which inhibits crystal growth because of the significant reduction in the number of kinks, thus degrading the crystal quality [10].

By varying the strength of the step–step attraction, a faceting

diagram was constructed [7] based on a singularity in the surface tension (Fig. 1). The surface tension is discontinuous around the (111) surface for $T < T_{f,1}$; the surface tension is discontinuous around the (001) surface for $T < T_{f,2}$. The step-faceting zone represents the temperature range $T < T_{f,2}$, the step droplet zone represents the range $T_{f,2} \leq T < T_{f,1}$, and the Gruber–Mullins–Pokrovsky–Talapov (GMPT) [11] zone represents the range $T_{f,1} \leq T$.

In the present work, we consider how the roughening transition on the (001) surface affects the morphology of the crystal and the locally merged steps. In the step droplet zone, the surface tension is continuous near the (001) surface, whereas it is discontinuous around the (111) surface. This discontinuity reflects the formation of locally merged steps. We will consider two cases in detail: a typical example of step droplet zone I ($\epsilon_{\text{int}}/\epsilon = -1.5$ and $k_B T/\epsilon = 1.0$), and a typical example of step droplet zone II ($\epsilon_{\text{int}}/\epsilon = -1.5$ and $k_B T/\epsilon = 1.4$).

2. p-RSOS model

The microscopic model considered here is the restricted solid-on-solid (RSOS) model with the point-contact-type step–step attraction (p-RSOS model). Here, “restricted” means that the height difference between any two neighboring lattice sites is restricted to values of $\{\pm 1, 0\}$. Point-contact-type step–step attraction refers to the attraction caused by the energy gain for a bonding state formed by overlapping orbitals at the meeting point of neighboring steps.

In the p-RSOS model, the Hamiltonian for the (001) surface can be written as follows:

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¹ In general, an ECS is similar to the Andreev (surface) free energy [2] (see the caption of Fig. 2 for more details). When the surface slope jumps at the facet edge on the ECS, this is referred to as a first-order shape transition after the fashion of a phase transition.

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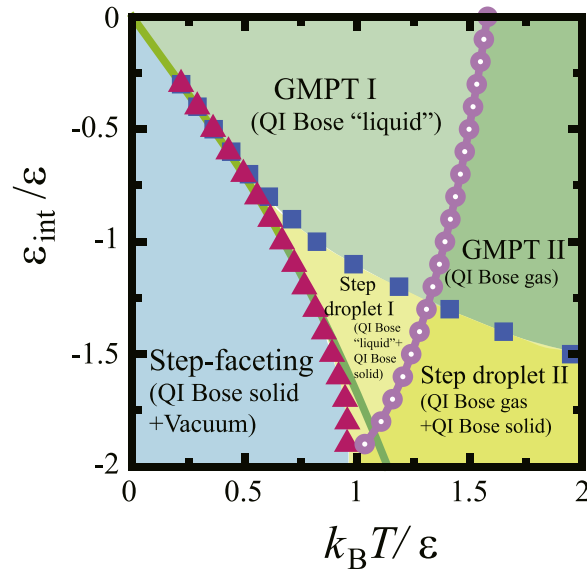


Fig. 1. Faceting diagram of the p-RSOS model for a vicinal surface obtained by the DMRG calculations. Squares: calculated points $T_{f,1}$. For $T < T_{f,1}$, the surface tension is discontinuous around the (111) surface. Triangles: calculated points $T_{f,2}$. For $T < T_{f,2}$, the surface tension is discontinuous around the (001) surface. Open circles: calculated roughening transition temperatures of the (001) surface. Solid line: zone boundary calculated using the two-dimensional Ising model. The definition of a QI Bose solid, QI Bose liquid, and QI Bose gas are given in a previous publication, from which this figure is taken [7].

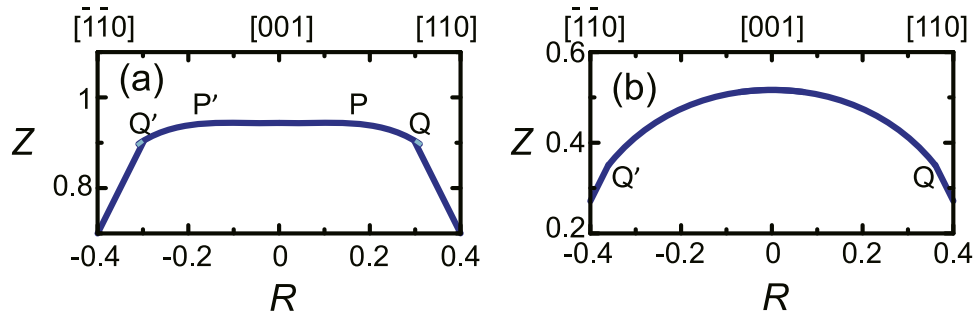


Fig. 2. Profile of the Andreev free energy, which is also the ECS profile. (a) $k_B T/\epsilon = 1.0$. Pale lines near Q and Q' indicate metastable surfaces. (b) $k_B T/\epsilon = 1.4$. $Z = \tilde{f}(\eta_x, \eta_y)/k_B T = \lambda z(x, y)/k_B T$, $R = \pm \sqrt{X^2 + Y^2}$ with $X = Y$, $(X, Y) = (\eta_x, \eta_y)/k_B T = -\lambda(x, y)/k_B T$, where $z(x, y)$ represents the ECS, and λ represents the Lagrange multiplier related to the crystal volume. We assume ϵ_{surf} is equal to ϵ . $\epsilon_{\text{int}}/\epsilon = -1.5$. The points P and P' indicate the (001) facet edge, and the points Q and Q' indicate the (111) facet edge.

$$\mathcal{H}_{\text{p-RSOS}} = \mathcal{N}\epsilon_{\text{surf}} + \sum_{n,m} \epsilon[|h(n+1, m) - h(n, m)| + |h(n, m+1) - h(n, m)|] + \sum_{n,m} \epsilon_{\text{int}}[\delta(|h(n+1, m+1) - h(n, m)|, 2) + \delta(|h(n+1, m-1) - h(n, m)|, 2)], \quad (1)$$

where \mathcal{N} is the total number of lattice points, ϵ_{surf} is the surface energy per unit cell on the planar (001) surface, ϵ is the microscopic step energy, $\delta(a, b)$ is the Kronecker delta, and ϵ_{int} is the microscopic step-step interaction energy. The summation with respect to (n, m) is performed over all sites on the square lattice. The RSOS condition is implicitly required. When ϵ_{int} is negative, the step-step interaction becomes attractive (sticky steps).

In order to evaluate a vicinal surface, we add the terms for the Andreev field [2]: $\boldsymbol{\eta} = (\eta_x, \eta_y)$ in order to introduce a step in the surface; note that this is an external field, similar to the chemical potential in a gas-liquid system. The adjusted Hamiltonian for the vicinal surface is [12]:

$$\mathcal{H}_{\text{vicinal}} = \mathcal{H}_{\text{p-RSOS}} - \eta_x \sum_{n,m} [h(n+1, m) - h(n, m)] - \eta_y \sum_{n,m} [h(n, m+1) - h(n, m)]. \quad (2)$$

From statistical mechanics, the (grand) partition function \mathcal{Z} is calculated as follows: $\mathcal{Z} = \sum_{\{h(m, n)\}} e^{-\beta \mathcal{H}_{\text{vicinal}}}$ where $\beta = 1/k_B T$. The summation with respect to $\{h(m, n)\}$ is taken over all possible values

of $h(m, n)$. The Andreev free energy $\tilde{f}(\boldsymbol{\eta})$ [2] is the thermodynamic (grand) potential calculated from the partition function \mathcal{Z} , as follows [12]:

$$\tilde{f}(\boldsymbol{\eta}) = \tilde{f}(\eta_x, \eta_y) = - \lim_{\mathcal{N} \rightarrow \infty} \frac{1}{\mathcal{N}} k_B T \ln \mathcal{Z}, \quad (3)$$

where \mathcal{N} is the number of lattice points on the square lattice.

As mentioned in the introduction, in low-dimensional cases, it is necessary to have more precision than that provided by a mean field calculation of the partition function. Fortunately, since the Hamiltonian is quite simple, we can map the p-RSOS model to a 19-vertex model [5] and then use the transfer matrix method to calculate it. We note that the transfer matrix version of the DMRG method, which is known as the product wave-function renormalization group (PWFRG) method [9], provides a way to efficiently calculate the largest eigenvalue of the transfer matrix.

Examples of the Andreev free energy calculated by the DMRG method are shown in Fig. 2 as a function of $(\eta_x/k_B T, \eta_y/k_B T)$ for $\eta_x = \eta_y$.

3. Shape transitions around the (001) and (111) surfaces: DMRG calculations

One of the effects of the roughening transition on the (001) surface $T_R^{(001)}$ is a change in the crystal habit. In Fig. 2, we show the calculated ECS around the (001) facet for $T < T_R^{(001)}$ (step droplet zone I) and

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