The Equilibrium Facet Shape of the Staggered Body-Centered-Cubic Solid-on-Solid Model
— A Density Matrix Renormalization Group Study —

Noriko Akutsu$^{1,*}$ and Yasuhiro Akutsu$^{2,**}$

$^1$Faculty of Engineering, Osaka Electro-Communication University, Neyagawa 572-8530, Japan
$^2$Department of Physics, Graduate School of Science, Osaka University, Toyonaka 560-0043, Japan

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We present a new method for the numerical calculation of the equilibrium crystal shape around a facet. Our method is based on the transfer matrix method with the product-wave-function renormalization group (PWFRG) algorithm for the asymmetric density matrix, which is an extension of the density matrix renormalization group (DMRG) algorithm. By applying this method to the staggered body-centered-cubic solid-on-solid model, which is known to exhibit the inverse roughening phenomena, we obtain the facet shape, shape exponents, and step tension.

§1. Introduction

The equilibrium crystal shape (ECS) is the shape of a crystal with the minimum surface free energy under a fixed volume constraint. The ECS consists of small planes, called facets, and curved regions that surround the facets (see Fig. 1). Because the ECS is a direct consequence of the anisotropic surface tension, information concerning the ECS is important for constructing micro-scale and nano-scale objects for electronic devices using the “self-organization” technique.

Theoretically, the ECS is interesting in itself, because it undergoes “faceting transition” accompanied by roughening transition of surfaces. The faceting transition is a shape transition, which occurs at the roughening transition temperature $T_R$ of a surface with low Miller index: For temperatures $T$ lower than $T_R$, the facet exists, and the surface of the planar facet is “smooth”, whereas for temperatures higher than $T_R$, the facet does not exist.

Moreover, for temperatures lower than $T_R$, the vicinal surface, which is slightly tilted with respect to the facet, exhibits universal behavior of the one-dimensional

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$^*$ E-mail: nori@phys.osakac.ac.jp
$^{**}$ E-mail: acts@phys.sci.osaka-u.ac.jp
Fig. 2. A facet and a vicinal surface. The enlargement in the upper right is an “atomic scale” view of the surface near the facet contour in the curved region, which can be regarded as an assembly of steps forming a vicinal surface.

_free fermion_ class if we regard the surface steps as linear elementary excitations in the facet plane.\(^{28)−41)}\) Since the surface of a facet is smooth, the vicinal surface is described by the terrace-step-kink (TSK) picture (see Fig. 2). The universal behavior of the vicinal surface is also known as the Gruber-Mullins-Pokrovsky-Talapov (GMPT)\(^{41)−51)}\) behavior.

The universal behavior of the vicinal surface has been established by exact calculations using the body-centered-cubic solid-on-solid (BCSOS) model.\(^{26),16)}\) Employing staggered body-centered-cubic solid-on-solid (st-BCSOS) models, the phenomena of inverse-roughening,\(^{52)}\) the disordered flat phase,\(^{53)−55)}\) and the reconstructed rough phase\(^{54),55)}\) have been studied. The st-BCSOS models are regarded as models of the (001) surface of the CsCl crystal in an electric field. In such models, the temperature dependence of the facet shape is of interest.

In this paper, we study the facet shape of the st-BCSOS model of Luijten et al.\(^{52)}\) [or the staggered F (st-F) model].\(^{56),57)}\) In order to obtain the facet shape, we adopt a new numerical calculational procedure. This procedure is based on the transfer matrix method with the product-wave-function renormalization group (PWFRG) algorithm\(^{58)−61)}\) for an asymmetric density matrix.\(^{62)}\) The PWFRG method is a variant of the density matrix renormalization group (DMRG) algorithm\(^{63),64)}\) developed for application to quantum spin systems.

This paper is organized as follows. We explain the staggered body-centered-cubic solid-on-solid (st-BCSOS) model in §2. In §3, we present the new calculational procedure for the equilibrium crystal shape (ECS) with the thermodynamics of the ECS. The mapping of the st-BCSOS model to a vertex model and the construction of the transfer matrix are also explained there. In §4, we study the universal behavior around the facet contour for the ECS. In §5, numerical results, including facet shapes and universal shape exponents, obtained using the transfer matrix method with the product-wave-function renormalization group (PWFRG) algorithm are presented. A summary and discussion are given in §6.
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Fig. 3. (a) Top view of the (001) surface of the CsCl lattice structure. (b) Two plaquettes, A and B. (c) The vertices corresponding to the plaquettes shown in (b). The vertex represented by the solid lines corresponds to the plaquette A, and that represented by the dotted lines corresponds to the plaquette B. The variables assigned to the legs of a vertex satisfy $u' + t' = u + t$.

Fig. 4. The six vertices and the assigned energies of the st-BCSOS model. The numbers, 0, 1/2, and 1, in the figure of vertices indicate the relative local heights on the surface.

§2. A staggered BCSOS model

We present the top view of a flat (001) surface of a CsCl crystal structure in Fig. 3(a). The height of the surface layer with the open circles is higher/lower than that of the surface layer with the closed circles by 1/2 of the lattice constant. From the figure, we can see that there are two kinds of “plaquettes”, which we designate A and B [Fig. 3(b)]. We assign the difference in height between nearest neighbor sites, which are denoted $u'$, $t'$, $u$, and $t$, to each endpoint of each leg of a vertex [Fig. 3(c)]. Note that we have the condition $u' + t' = u + t$. These vertices are mapped to the st-BCSOS system of Luijten and van Beijeren, as shown in Fig. 4.\(^{52}\)

Physically, the (001) surface of the CsCl-type crystal is a kind of “polar surface”, because the surface has a double layer structure, like the (111) surface of the GaAs crystal. With the external electric field normal to the surface (001), the surface energy of the surface layer of the open circles is different form that of the surface layer of the closed circles. This surface energy difference relates to $s$ in Fig. 4. On the other hand, (111) surfaces of the CsCl-type crystal is not the “polar surface”, because the surface has a single layer structure. The surface energy of (111) surface relates to $\epsilon$ in Fig. 4.

Let us express the set of values $u'$, $t'$, $u$, and $t$ as $((u',t'),(u,t))$. Then, the statistical weights of the plaquettes A and B [Fig. 3(b)] are given as follows:

$$w_A \left( \left( \frac{1}{2}, \frac{1}{2} \right), \left( \frac{1}{2}, \frac{1}{2} \right) \right) = w_B \left( \left( \frac{1}{2}, \frac{1}{2} \right), \left( \frac{1}{2}, \frac{1}{2} \right) \right)$$
where $\epsilon$ and $s$ are the energies assigned in Fig. 4.

§3. Calculation of the equilibrium crystal shape

3.1. Transfer matrix for the (001) surface of the CsCl crystal structure

The partition function of the st-BCSOS model is obtained using the transfer matrix method. Corresponding to the unit cell structure of the surface [Fig. 3(a)], which contains two atoms in a cell, the unit cell of the transfer matrix is that shown in Fig. 5(a). The unit cell of the transfer matrix is represented by the diagram of the square with two legs on each side appearing in Fig. 5(b). Therefore, the transfer matrix is given by the connected diagrams, as shown in Fig. 5(c).

In order to apply the transfer matrix method to the vicinal surface, we add terms containing the Andreev field, $\eta = (\eta_x, \eta_y)$, which is a thermodynamic field that acts...
to make surface tilt, to the statistical weight of each vertex as

$$\sum_{i=1}^{N} (-\Delta_{x,i} \eta_x - \Delta_{y,i} \eta_y),$$  \quad (3.1)

where $N$ is the linear size of the system in the horizontal direction, and $\Delta_x$ and $\Delta_y$ are the surface height differences in the $x$ direction and $y$ direction, respectively. Let us define the local slope as $(\Delta_x, \Delta_y)$, with $\Delta_x = (u'_x + t)/2$ and $\Delta_y = (u + t')/2$. From Eqs. (3.1) and (2.1), we assign the statistical weights of the vertices for the vicinal surface as follows:

$$\tilde{w}_A((u', t'), (u, t)) = w_A((u', t'), (u, t)) \times \exp \left[ (\Delta_x \eta_x + \Delta_y \eta_y) / k_B T \right],$$

$$\tilde{w}_B((u', t'), (u, t)) = w_B((u', t'), (u, t)) \times \exp \left[ (\Delta_x \eta_x + \Delta_y \eta_y) / k_B T \right].$$  \quad (3.2)

The partition function $Z(\beta \eta_x, \beta \eta_y)$, where $\beta = 1/k_B T$, for a large system size is obtained as

$$Z(\beta \eta_x, \beta \eta_y) = \text{Tr} \hat{T}^M, = A_T^M,$$  \quad (3.3)

where $M$ is the linear size of the system in the vertical direction, and $A_T$ is the largest eigenvalue of the transfer matrix. The Andreev free energy $\tilde{f}(\eta)$ is calculated from the partition function $Z$ as

$$\beta \tilde{f}(\eta) = - \lim_{M,N \to \infty} \frac{1}{MN} \ln Z.$$  \quad (3.4)

The mean surface slope in the $x$ direction is calculated from the equation

$$p_x = \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \langle \Delta_{x,i} \rangle,$$  \quad (3.5)

where, the angular brackets represent the thermal average.

For the diagonalization of the transfer matrix, we adopt the PWFRG algorithm. The largest eigenvalue of transfer matrix and its bases in the thermodynamic limit are obtained at the fixed point of the PWFRG iteration.

In order to apply the PWFRG method to the calculation of the ECS, we have to use the PWFRG algorithm for the asymmetric density matrix. The existence of the term $\eta_y \Delta y$ in the statistical weight of the vertex breaks the symmetry between the “right” projection operator and the “left” projection operator in the PWFRG algorithm. We, therefore, perform the PWFRG calculation for the asymmetric case according to the procedure described in Ref. 62).

3.2. Thermodynamics of the ECS

There are several phenomenological methods for obtaining the ECS from the anisotropic surface tension, including the Wulff construction based on the Wulff theorem, Frank’s F-figure method, and the Landau-Andreev method. We now give a brief explanation of the Landau-Andreev method.
Let us consider a facet and its neighboring curved surface of the ECS with mesoscopic size. We use the Cartesian coordinates \((x, y, z)\) with the \(z\) direction chosen to be normal to the facet, which allows us to describe the ECS by the equation \(z = z(x, y)\) (see Fig. 1). The surface gradient vector \(\mathbf{p} = (p_x, p_y)\) at the position \((x, y, z(x, y))\) is defined by \(p_x = \partial z/\partial x\) and \(p_y = \partial z/\partial y\). By \(f(\mathbf{p})\) we denote the free energy per unit projected area \(^7\) of the surface with fixed surface gradient \(\mathbf{p}\). Then, the variational equation for the shape of the minimum total surface free energy under the condition of fixed volume becomes

\[
\begin{align*}
-\lambda z(x, y) &= f(\mathbf{p}) - p_x \frac{\partial f}{\partial p_x} - p_y \frac{\partial f}{\partial p_y}, \\
\lambda x &= -\frac{\partial f(\mathbf{p})}{\partial p_x}, \quad \lambda y = -\frac{\partial f(\mathbf{p})}{\partial p_y},
\end{align*}
\] (3.6)

where \(\lambda\) is the Lagrange multiplier corresponding to the fixed volume condition.

Here we introduce the “Andreev field” \(^{12}\) \(\eta = (\eta_x, \eta_y)\) as

\[
\eta_x = \frac{\partial f(\mathbf{p})}{\partial p_x}, \quad \eta_y = \frac{\partial f(\mathbf{p})}{\partial p_y}.
\] (3.7)

This Andreev field consists of the thermodynamic variables conjugate to the surface gradient, and it is equivalent to the Andreev field introduced in the previous section. Comparing Eq. (3.7) with Eq. (3.8), we have

\[
-\lambda x = \eta_x, \quad -\lambda y = \eta_y.
\] (3.8)

Using the Andreev field, we perform the Legendre transformation of \(f(\mathbf{p})\) as

\[
\tilde{f}(\eta) = f(\mathbf{p}) - \eta \cdot \mathbf{p}.
\] (3.9)

Comparing Eq. (3.9) with Eq. (3.6), we have

\[
-\lambda z(\mathbf{r}) = \tilde{f}(-\lambda \mathbf{r}),
\] (3.10)

where \(\mathbf{r} = (x, y)\) is the position vector, with the relationship \(\eta = -\lambda \mathbf{r}\) (see Eq. (3.9)). In what follows, we consider the “normalized” ECS by setting \(\lambda = -1\) in Eq. (3.9) and Eq. (3.10). Therefore, we can obtain the normalized ECS directly if we calculate \(\tilde{f}(\eta)\) as a function of \(\eta_x\) and \(\eta_y\).

3.3. Calculation of the ECS using the transfer matrix method

In the transfer matrix method, the Andreev free energy is directly obtained as a function of \((\eta_x, \eta_y)\) [Eq. (3.4)]. As shown in Eqs. (3.9) and (3.10), \(\tilde{f}(\eta)\) gives the normalized ECS. In the PWFRG calculation, the facet edge \(x_c(y)\) is determined as the point where \(p_x\) decreases to zero on the \(p_x-x\) curve with fixed \(y_c\) (see Fig. 6). Therefore, the curve \(\{(x_c(y_c), y_c)\}\) is the facet contour corresponding to the zero-gradient limit of the curved region.
§4. Universal behavior of the equilibrium crystal shape

4.1. Surface free energy in the universal form

For temperatures lower than $T_R$, the vicinal surface is described by the TSK picture. Regarding the steps as the linear elementary excitations in the facet plane, the surface free energy per unit projected area for the vicinal surface is derived in the 1D free fermion form\textsuperscript{28)−30) or GMPT\textsuperscript{42), 41)} form as follows:

$$f(p) = f(0) + \gamma(\theta) \frac{|p|}{d} + B(\theta) \frac{|p|^3}{d^3} + O(|p|^4). \quad (4.1)$$

Here, $f(0)$ is the surface tension of the facet-plane, $\gamma(\theta)$ is the step tension (step free energy per unit length), $\theta$ is the angle of the mean running direction of steps on the vicinal surface (see Fig. 2), $d (= 1)$ is the height of a single step, and $B(\theta)$ is the step interaction coefficient. The surface gradient $p = (p_x, p_y)$ is given in terms of $\theta$ as $(|p| \cos \theta, |p| \sin \theta)$.

4.2. Equilibrium facet shape

From the universal form of $f(p)$ given in Eq. (4.1), together with the thermodynamic equations (3.8) and (3.9), we obtain the following equations near the facet edge in the curved region [omitting $O(|p|^4)$ and higher-order terms]:\textsuperscript{32) }

$$x = x_c(\theta) + |p|^2 [3B(\theta) \cos \theta - B'(\theta) \sin \theta], \quad (4.2)$$
$$y = y_c(\theta) + |p|^2 [3B(\theta) \sin \theta + B'(\theta) \cos \theta], \quad (4.3)$$

with

$$B'(\theta) = \partial B(\theta) / \partial \theta, \quad (4.4)$$

where the curve $\{(x_c(\theta), y_c(\theta))\}_\theta$ is the facet contour corresponding to the zero-gradient limit of the curved region (see Figs. 2, and 6). Explicitly, we have

$$x_c(\theta) = \gamma(\theta) \cos \theta - \gamma'(\theta) \sin \theta, \quad (4.5)$$
$$y_c(\theta) = \gamma(\theta) \sin \theta + \gamma'(\theta) \cos \theta, \quad (4.6)$$
with
\[ \gamma'(\theta) = \partial \gamma(\theta)/\partial \theta. \] (4.7)

We should note that (4.5) and (4.6) are precisely the equations determining the two-dimensional (2D) ECS (i.e., facet shape) from \( \gamma(\theta) \), regarded as a one-dimensional interface tension.\(^{32}\)

### 4.3. Shape exponents

In this subsection, we choose the \( x \) and \( y \) axes to be parallel to the directions of the principal curvatures in order to explain the universal values of the shape exponents clearly. Then, we generalize the direction of the \( x \) and \( y \) axes again to obtain the general expressions for the profile of the ECS with the shape exponents.

For a given ECS described by the equation \( z = z(x, y) \), we specify any point on the ECS surface by the two-dimensional position vector \((x, y)\). For convenience, we take the \( xy \) plane with \( z = 0 \) to be the facet plane, which corresponds to setting \( f(0) = 0 \) in (4.1). Let us fix a point \( P \) on the facet contour and choose the \( x \) and \( y \) axes so that the \( y \) axis is parallel to the line tangent to the facet contour at \( P \), and the \( x \) axis is perpendicular to it (Fig. 7). With this choice of the coordinate system, we have \( \theta = 0 \) at \( P \) and \( \gamma'(0) = 0 \) [see (4.6)]. Our task is to obtain the ECS profile close to the point \( P = (x_c(0), y_c(0)) = (x_c(0), 0) \).

Along the \( x \) axis \([\theta = 0, \Delta x \equiv x - x_c(0)]\), from (4.2) and (4.3) we have

\[ |p| = p_x = \frac{1}{\sqrt{3B(0)}}(\Delta x)^{1/2}, \] (4.8)

giving the “normal” profile, with the well-known exponent \( \theta_x = 3/2 \):

\[ z = \frac{2}{3\sqrt{3B(0)}}|\Delta x|^{3/2}. \] (4.9)

The profile (4.9) leads to divergent behavior of the normal curvature \( \kappa_x \approx \partial^2 z/\partial x^2 \sim (\Delta x)^{-1/2} \) near the facet edge. Due to the universal Gaussian curvature jump at the facet edge,\(^{33}\) the “tangential curvature” \( \kappa_y \approx \partial^2 z/\partial y^2 \), along the \( x \) axis vanishes\(^{33}\) as \((\Delta x)^{1/2}\). [The Gaussian curvature is the product of the two principal curvatures, \( \kappa_x \) and \( \kappa_y \) (see Appendix A).]

We should note that a different exponent \( \theta_y > 2 \) for the tangential profile \( z \sim (\Delta y)^{\theta_y} [\Delta y = y - y_c(0)] \) is implied by the vanishing of the tangential curvature at \( P \).

The actual value of \( \theta_y \) can be derived as follows. Note that along the tangential line \([x - x_c(0) = 0], \theta \) and \(|p| \) are not independent but, instead, must satisfy the relation

\[ -\frac{1}{2} \tilde{\gamma}(0) \theta^2 + 3B(0)|p|^2 = 0, \] (4.10)

[Fig. 7. Choice of the \( x \) and \( y \) axes at \( P \) on the facet contour. The \( y \) axis is parallel to the tangential line at the point \( P \).]
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where we have $\bar{\gamma}(0) = \bar{\gamma}(\theta)|_{\theta=0}$, and $\bar{\gamma}(\theta) = \gamma(\theta) + \partial^2 \gamma(\theta)/\partial \theta^2$ is the step stiffness. Equation (4.10) can be derived by expanding (4.2) and (4.5) with respect to $\theta$ and $|p|$.(Note that $|p| \ll 1$ and $|\theta| \ll 1$, very near the point $P$.) Combining (4.10) with (4.2)–(4.6), we obtain

$$\theta = \frac{\Delta y}{\bar{\gamma}(0)},$$  (4.11)

$$|p| = \frac{\Delta y}{\sqrt{6\bar{\gamma}(0)B(0)}}$$  (4.12)

along the $y$ direction. Near $P$, $z = \bar{f}(x_c(0), \Delta y + y_c(0))$ can be expanded as

$$-z = [\gamma(0) + \frac{1}{2} \gamma''(0) \theta^2]|p| + B(0)|p|^3$$

$$-\Delta y |p| \theta - x_c(0)|p| \left(1 - \frac{1}{2} \theta^2\right).$$  (4.13)

Substituting (4.11) and (4.12) into (4.13), we have

$$z = \frac{1}{3\sqrt{6B(0)\bar{\gamma}(0)^2}}|\Delta y|^3,$$  (4.14)

giving $\theta_y = 3$ (see Appendix B for details). We should remark here that the results (4.9) and (4.14) apply to any point on the facet contour, because the point $P$ has been chosen arbitrarily. Hence, $\bar{\gamma}(0)$ and $B(0)$ in (4.9) and (4.14) can be replaced by $\bar{\gamma}(\theta)$ and $B(\theta)$.

In systems with only short-range inter-step interactions, like the st-BCSOS model, the coefficient $B(\theta)$ is universally given by $^{33}$

$$B(\theta) = \frac{\pi^2(k_B T)^2}{6\bar{\gamma}(\theta)}.$$  (4.15)

Therefore, the step interaction coefficients in $f(p)$ given by Eq. (4.1) is determined by the step stiffness. Substituting the universal relation Eq. (4.15) into Eqs. (4.2) and (4.14), we have

$$|p_x| = \frac{\sqrt{2\beta \bar{\gamma}(0)}}{\pi} [\beta|x - x_c(0)|]^{1/2},$$  (4.16)

$$|p_y| = \frac{1}{\pi \beta \bar{\gamma}(0)} (\beta y)^2,$$  (4.17)

where $\beta = 1/k_B T$ (see Appendix C).

In the case that the $y$ axis intersects the tangential line at the point $P$ at an angle $\theta_0$, we have

$$p_x = \cos^2 \frac{3}{2} \theta_0 \sqrt{\frac{|x - x_c(\theta_0)|}{3B(\theta_0)}},$$  (4.18)

and

$$p_y = \sin^2 \frac{3}{2} \theta_0 \sqrt{\frac{|y - y_c(\theta_0)|}{3B(\theta_0)}},$$  (4.19)

in the curved region near the facet contour on the ECS.
§5. PWFRG results

5.1. Free fermion limit

To elucidate the accuracy of the transfer matrix method with the PWFRG algorithm, we have studied the exactly soluble case of the st-BCSOS model (the free fermion limit) with \( k_B T_{FF}/\epsilon = 2/\ln 2 \) and \( s/\epsilon = 2.57 \).

The exact form of the \( D \) function \(^{22}\) in the st-F model was derived by Baxter \(^{57}\) as

\[
D(\omega_x, \omega_y) = M - 2 \cosh \omega_x \cosh \omega_y, 
\tag{5.1}
\]

where \( \omega_x = \beta y, \omega_y = \beta x, M = 2 \cosh S, \) and \( \beta = 1/k_B T \). Here, \((x, y)\) corresponds to \((\eta_x, \eta_y)\) with \( \lambda = -1 \), and \( S \) corresponds to \( 4\beta \epsilon \) in the free fermion limit. The \( D \) function is the determinant of the connectivity matrix of the two-dimensional free random walk, which describes the surface step zigzag structure. The equilibrium facet shape is given by the zeros of the \( D \) function. \(^{22}\) Then, the explicit form of the equilibrium facet shape is

\[
2 \cosh \beta x \cosh \beta y = M, 
\tag{5.2}
\]

where \( M = 17/4 \). The Andreev field dependence of the surface slope \( p_x \), which is proportional to the polarization derived in Ref. 57), is known to be (at \( y = 0 \))

\[
p_x = \frac{1}{\pi} \arccos\{M/[2 \cosh(x/k_B T)]\}, 
\tag{5.3}
\]

where we denote \((\eta_x, \eta_y)\) as \((x, y)\).

![Fig. 8. The free fermion limit of the st-BCSOS model (exactly soluble case). Here, \( k_B T_{FF}/\epsilon = 2/\ln 2 \) and \( s/\epsilon = 2. \) Also, we have \( \eta_x = -\lambda x \) and \( \eta_y = -\lambda y \) (\( \lambda = -1 \)). The open circles represent the results of the PWFRG calculations. (a) \( p_x \) vs \( \eta_x/k_B T \) at \( \eta_y = 0 \). The solid curve is the exact curve, given by Eq. (5.3). The number of retained bases \( m \) in the DMRG/PWFRG terminology is 20 or 28. (b) The equilibrium facet shape. The solid curve is the exact facet shape, given by Eq. (5.2). The number of retained bases \( m \) is 12 or 13. The PWFRG calculation is carried out in the region satisfying \( \eta_x \geq 0 \) and \( \eta_y \geq 0 \). From the symmetry of the lattice, the PWFRG values are valid everywhere on the facet contour.](image-url)
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In Fig. 8(a), we plot with open circles $p_x$ as a function of $\beta x$ for $y = 0$, calculated using the transfer matrix method with the PWFRG algorithm. We have found that the PWFRG gives a $p_x-\beta x$ curve that is close to the exact one.

The location of the facet contour $x_c(y)$ with fixed $y$ (see Fig. 6) is obtained from the $p_x$ curve calculated using the PWFRG method for each $y$. In order to obtain a more precise value of $x_c(y)$, we have carried out a least square fitting to the $p_x-\beta x$ curve for small $p_x$ by employing the fitting equation

$$\beta x = A_1 + A_2 p_x^2 + A_3 p_x^3.$$  (5.4)

Then, $\beta x_c(y)$ is obtained as the value of $A_1$. The calculated $(\beta x_c, \beta y_c)$ are displayed in Fig. 8(b). The solid curve is the exact one, given by Eq. (5.2). From the figure, we can see that the facet shape obtained using PWFRG agrees with the exact one.

One of the merits of the PWFRG method is that with it we are able to obtain the free energy. In Fig. 9, we plot the $\eta_x/k_B T$ dependence of the Andreev free energy for $\eta_y/k_B T = 0$, $\eta_y/k_B T = 0.5$, and $\eta_y/k_B T = 1.0$ obtained from Eq. (3.4). In the figure, from Eqs. (3.9) and (3.11) with $\lambda = -1$, the vertical axis and the horizontal axis correspond to $(z/k_B T)^{2/3}$ and $(x/k_B T)$, respectively. From the figure, for the shape exponent we find $\theta_x = 3/2$ not only for $\eta_y/k_B T = 0$ but also for $\eta_y/k_B T = 0.5$, and $\eta_y/k_B T = 1.0$, which confirms Eq. (4.18).

5.2. A case in the region of normal roughening

The phase diagram of the st-BCSOS model is given in Fig. 3 of Ref. 52). As a non-solvable example in the normal roughening region, we choose the point $k_B T/e = 0.75 \ln 2$, $s/\epsilon = 2$ in the phase diagram. In the case $\epsilon > 0$, at low temperatures, the (001) surface becomes “smooth”, and the Wulff figure has a cusp in the direction of the (001) surface.

In Fig. 10, we show the calculated facet shape and the $p_x^2-\beta x$ lines for several values of $y$. As seen from Fig. 10(a), the shape obtained using the PWFRG agrees well with the solid curve. The solid curve is given by Eq. (5.2) with $M =$.

Fig. 9. The universal behavior of the ECS in the free fermion limit (exactly soluble case). Here, $k_B T_{FF}/\epsilon = 2/\ln 2$ and $s/\epsilon = 2$. The open circles represent the PWFRG results. The number of retained bases is $m = 12$ or 13. The three plots correspond to $\eta_y/k_B T = 0$, $\eta_y/k_B T = 0.5$, and $\eta_y/k_B T = 1.0$, from right to left.
Fig. 10. The case in the normal roughening region. Here, $\epsilon/k_BT = (3/4) \ln 2$ and $s/\epsilon = 2$. Also, we have $\eta_x = -\lambda x$ and $\eta_y = -\lambda y$ ($\lambda = -1$). The number of retained bases is $m = 17, 21$ or $24$. (a) The equilibrium facet shape. The open circles represent the PWFRG calculations, and the solid curve represents Eq. (5·2) with $M = 11.3638$. (b) $p_x^2$ vs $\eta_x/k_BT$. From right to left, we have $\eta_y/k_BT = 0, 0.5, 1.0$.

Fig. 11. The universal behavior in the normal roughening region. Here, we have $\epsilon/k_BT = (3/4) \ln 2$ and $s/\epsilon = 2$. The closed squares represent the PWFRG calculation. The number of retained bases is $m = 17, 21$ or $24$. (a) $p_y$ along the tangential line $\eta_x = \eta_{xc}(0) = -\lambda x_c(0) = 2.4226k_BT$ ($\lambda = -1$). (b) $(\eta_{yc}/k_BT)^2$ vs $2.4226 - \eta_{xc}/k_BT$ along the facet contour. In this plot, the lines are simply drawn to connect the calculated points.

$11.364 \pm 0.003$, which is estimated from the $x_c(0)$ value obtained with the PWFRG calculation.

From Fig. 10(b), we can see the GMPT-type universal behavior of Eq. (4·8) not only for $y = 0$ but also for $y \neq 0$. In this case too, the shape exponent is given by $\theta_x = 3/2$. Since the step stiffness $\tilde{\gamma}(\theta)$ increases rapidly as a function of $\theta$, we find
from Eqs. (4.18) and (4.15) that the slopes of the lines become larger as $y$ increases.

In order to study the shape exponent $\theta_y$, we calculate $p_y$ along the tangential line of the facet contour. In Fig. 11(a), we plot the $p_y-(\beta y)^2$ curve. From the figure, we can see that the curve is linear in the region of small $\beta \eta_y$, and we obtain $\theta_y = 3$.

To confirm the consistency, we calculate $\beta \tilde{\gamma}(0)$ from the figures. From Fig. 10 (b), we obtain $\beta \tilde{\gamma}(0) = 0.976 \pm 0.002$ from the least square fitting parameter $A_2$ of

$$\beta x = A_1 + A_2 p_x^2 + A_3 p_x^3 + A_4 p_x^4. \quad (5.5)$$

The value $\beta \tilde{\gamma}(0) = 0.95 \pm 0.05$ is obtained from the slope of the $p_y-\beta y$ curve for small $p_y$ ($p_y < 0.01$) at $\beta x_c = 2.4226$ [Fig. 11(a)] with Eq. (4.17). In addition, we give the $(\beta \Delta y)^2 - \beta \Delta x$ curve. From the slope of the curve in the Fig. 11(b) for small $\eta_{yc}/k_BT$ $[(\eta_{yc}/k_BT)^2 < 0.4]$ with Eq. (B.1), we obtain $\beta \tilde{\gamma}(0) = 0.990 \pm 0.015$. Therefore, we concluded that the numerical values of $\beta \tilde{\gamma}(0)$ we have obtained are consistent with each other.

5.3. A case in the inverse roughening region

In the case $\epsilon < 0$, it is conjectured that inverse roughening phenomena appear. In this section, we study the facet shape and the universal behavior in such a case. We choose the point $s/k_BT = 0.4$, $\epsilon/s = -1.1$ in the phase diagram of Fig. 3 in Ref. 52).

In order to obtain the facet contour $x_c(y_c)$, we have carried out a least square fitting for the $p_x-\beta x$ curve in Eq. (5.5). In Fig. 12 (a), we present the facet shape. It is seen that the shape is almost circular. The facet contour calculated using the PWFRG method agrees with the curve obtained using Eq. (5.2) with $M = 2.00036665$. (b) The $p_x^2-\eta_x/k_BT$ curve.

![Fig. 12. The case in the inverse roughening region. Here, $s/k_BT = 0.4$ and $\epsilon/s = -1.1$. Also, we have $\eta_x = -\lambda x$ and $\eta_y = -\lambda y$ ($\lambda = -1$). The open circles represent the PWFRG calculation. The number of retained bases is $m = 28$ or 32. (a) The equilibrium facet shape. The solid curve represents Eq. (5.2) with $M = 2.00036665$. (b) The $p_x^2-\eta_x/k_BT$ curve.](image-url)
Fig. 13. Tangential behavior around the facet contour in the inverse roughening region. Here, $s/k_B T = 0.4$ and $\epsilon/s = -1.1$. Also, we have $\eta_x = \eta_{xc}(0) = -x_c(0) = 0.0191465 k_B T$. The number of retained bases is $m = 32$.

Fig. 14. Inverse temperature dependence of the step tension. Here, $\epsilon/s = -1.1$ and $\epsilon < 0$. The open squares represent the PWFRG calculation. The number of retained bases is $m = 32$ or 28. The lines are drawn simply to connect the open squares.

$2.000367 \pm 0.000005$. Because the temperature is near the roughening transition temperature, the size of the facet is small, which implies small values of $\beta x_c$, $\beta y_c$, and $\beta \gamma$.

We plot the $p_x^2 - \beta \eta_x (\beta = 1/k_B T)$ curve in Fig. 12(b). GMPT-type universal behavior is seen only in the region of small $p_x$, which is about 1/100 of the region shown in Fig. 10(b). In Fig. 13, we plot the tangential behavior of the facet contour. The linear part of $p_y$ is also seen for small $p_y (p_y < 0.001)$.

Along the line $\epsilon/s = -1.1$ ($\epsilon < 0$) in the phase diagram of Ref. 52), we calculate $\beta \gamma(0)$ ($= \beta x_c(0)$, $\lambda = -1$), which we denote $\beta \gamma$. In Fig. 14, we plot $\beta \gamma$ calculated using the PWFRG method. As seen from the figure, $\beta \gamma$ has a maximum value of approximately $\gamma/k_B T = 0.019$ at about $s/k_B T = 0.4$. The lower roughening transition temperature $T_{R-}$ along the line $\epsilon/s = -1.1$ is determined as $s/k_B T_{R-} = 1.63 \pm 0.07$, where the slope of $p_x - \beta x$ curve has the universal value $2/\pi$ in the limit $x \to 0$. Therefore, in the region $0.4 < \beta s < 1.63$, inverse roughening phenomena
The Equilibrium Facet Shape of the Staggered BCSOS Model

Chapter 6. Summary and discussion

We have presented a new numerical procedure to obtain the surface profile and the surface gradient of the equilibrium crystal shape (ECS) around a facet employing the transfer matrix method with the product-wave-function renormalization group (PWFRG) algorithm. We have also studied the shape exponents for the facet contour of the equilibrium crystal shape (ECS). We have shown that the profile \( z \sim (\Delta y)^{\theta_y} \) (where \( \Delta y \) is the distance along the tangential direction at the facet edge) with \( \theta_y = 3 \), which is a direct consequence of the Gruber-Mullins-Pokrovsky-Talapov (GMPT) type expansion of the surface free energy

\[
f(p) = f(0) + \gamma(\theta) |p|/d + B(\theta)|p|^3/d^3 + \ldots.
\]

We have applied the PWFRG method to the staggered body-centered-cubic solid-on-solid (st-BCSOS) model of the vertex energies presented in Ref. 52. The st-BCSOS model is regarded as a model of the (001) surface of the CsCl crystal structure. In order to determine the degree of precision of the PWFRG method, we applied the PWFRG method to the solvable case of the st-BCSOS model in the free-fermion limit \( k_B T_{FF}/\epsilon = 2/\ln 2, s/\epsilon = 2 \). The values calculated using the PWFRG method agree well with the exact ones in the cases that the number of “retained bases” is \( m = 12 – 28 \) in the terminology of the density matrix renormalization group (DMRG) method.

We have applied the PWFRG method to two non-solvable cases of the st-BCSOS model, that in the normal roughening region and that in the inverse roughening region. For the st-BCSOS model in the normal roughening region, where \( k_B T/\epsilon = 0.75 \ln 2 \) and \( s/\epsilon = 2 \), we have calculated the surface profile and the surface gradient of the ECS. Then we obtained a facet shape which agrees well with the shape given by Eq. (5.2) with \( M = 11.364 \pm 0.003 \). We have numerically confirmed the universal values of the shape exponents \( (\theta_x, \theta_y) \) to be \( (3/2, 3) \). We have estimated the step stiffness \( \tilde{\gamma}(0)/k_B T \) as \( 0.976 \pm 0.002 \) from the \( p_x-\eta_x/k_B T \) curve [Fig. 10(b)], \( 0.95 \pm 0.05 \) from the \( p_y-\eta_y/k_B T \) curve [Fig. 11(a)], and \( 0.990 \pm 0.015 \) from the \( (\eta_{yc}/k_B T)^2-(2.4226 - \eta_{xc}/k_B T) \) curve [Fig. 11(b)]. These are all consistent, within the uncertainties.

For the st-BCSOS model in the inverse roughening region, where \( s/k_B T = 0.4 \) and \( \epsilon/s = -1.1 \), we have carried out the PWFRG calculation for the surface profile around the facet. The calculated facet shape is almost circular, and agrees with the shape given by Eq. (5.2) with \( M = 2.000367 \pm 0.000005 \). Even in this case, the shape exponents have the universal values of the 1D free fermion class, though the universal behavior is seen only in the small \( |p| < 0.001 \) region around the facet contour (see Fig. 12).

We should make a remark about the “wing regions” of the reconstructed rough phase adjacent to the (001) facet, which were discovered by Carlon and van Beijeren in a mean field calculation of the ECS using the st-BCSOS model. Since the (001) surface of the CsCl-type crystal is a kind of “polar surface” and has a double layer structure, like the (111) surface of the GaAs crystal, there may be a step of
2n-mers or a 2n-body bound state \((n = 1, 2, 3, \cdots)\) with a height of \(2n \cdot d\). The origin of the “wing regions” of the reconstructed rough phase is believed to be the competition among the ledge energy, the external electric field, and the configurational entropy.

If the steps of a 2n-body bound state are formed, the assembly of the bounded steps\(^{65}\) exhibits the universal behavior \(f_{2n}(p) = f_{2n}(0) + \gamma_{2n}|p|/(2nd) + B_{2n}|p|^3/(2nd)^3 + O(|p|^4)\). Because \(\gamma_{2n} \sim \gamma(0) \cdot 2n\) and \(B_{2n} \sim B(0)/(2n)\), the amplitudes of \(|p|/d\) and \(|p|^3/d^3\) become \(\gamma(0)\) and \(B(0)/(2n)^4\), respectively. From Eqs. (4.9) and (4.14), where \(B(0)\) is replaced by \(B(0)/(2n)^4\), the profile of the facet contour for the 2n-body bounded steps is obtained. Furthermore, the emergence of the reconstructed rough phase of the ECS in the narrowed area suggests the bound-unbound transition of steps. The bound-unbound transition is known to occur if there are attractive interactions among steps.\(^{66}\)

In the model of Luijten et al.\(^{52}\) (that considered presently), attractive interactions are not introduced. The statistical weights of the vertices in the model of Luijten et al. are slightly different from those in the model of Carlon and van Beijeren. The complex competition, which also exists in the model of Luijten et al., leads to the inverse roughening phenomena. In the three cases for the profile of the ECS around the (001) facet that we have studied with PWFRG calculations, we do not obtain the “wing regions” nor evidence of the formation of bounded steps.

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Appendix A

Curvature Tensor

The first fundamental quantity,\(^{67,20}\) i.e., the induced covariant metric tensor \(g_{\mu\nu} (\mu, \nu = 1, 2)\) of the surface, is given by \(g_{\mu\nu} = \delta_{\mu\nu} + p_\mu \cdot p_\nu\), where \(\delta_{\mu\nu}\) is the Kronecker’s delta (\(\delta_{\mu\nu} = 1\) when \(\mu = \nu\) and \(\delta_{\mu\nu} = 0\) otherwise), \(p_1 = p_x\), and \(p_2 = p_y\).

The second fundamental quantity, \(H_{\mu\nu}\), is given by \(H_{\mu\nu} = -(1/\sqrt{g})\partial^2 z(x)/\partial x^\mu \partial x^\nu\), where \(g = \det(g_{\mu\nu})\), \(x^1 = x\) and \(x^2 = y\). The curvature tensor is the mixed tensor \((H^\nu_\mu)\), given by \(H^\nu_\mu = \sum_\alpha g^{\mu\alpha} \cdot H_{\alpha\nu}\), where \((g^{\mu\nu}) = (g_{\mu\nu})^{-1}\). The Gaussian curvature \(K\) is defined by \(K = \det H^\nu_\mu\).

In the limit \(|p| \to 0\), \(g_{\mu\nu}\) becomes \(\delta_{\mu\nu}\), and \(H^\nu_\mu\) reduces to \(H_{\mu\nu}\). As we pointed out in Ref. 20, \(H_{\mu\nu}\) can be written in terms the stiffness tensor \(f^{ij} = \partial^2 f(p)/\partial p_i \partial p_j\).
as

\[
(H_{ij}) = -\begin{pmatrix}
\frac{\partial^2 z}{\partial x^2} & \frac{\partial^2 z}{\partial x \partial y} \\
\frac{\partial^2 z}{\partial y \partial x} & \frac{\partial^2 z}{\partial y^2}
\end{pmatrix} = \lambda \begin{pmatrix}
\frac{\partial^2 f}{\partial p_x^2} & \frac{\partial^2 f}{\partial p_x \partial p_y} \\
\frac{\partial^2 f}{\partial p_y \partial p_x} & \frac{\partial^2 f}{\partial p_y^2}
\end{pmatrix}^{-1},
\]

(A.1)

where \(f(p)\) is the surface free energy per unit projected area, and \(\lambda\) is the Lagrange multiplier corresponding to the ECS.

Adopting Eq. (4.1) as the form of \(f(p)\), and taking account of Eqs. (3.6)–(3.8), together with Eqs. (4.2)–(4.6), we obtain the explicit forms of \(H_{\mu\nu}\) as follows:

\[
H_{11} = \frac{\lambda}{Q} \left\{ \tilde{\gamma} \cos^2 \theta / p \right\} 
+ p[(3B' - B'') \sin \theta \cos \theta + (3B + B'') \cos^2 \theta] 
+ 2p[3B \cos^2 \theta + B' \cos \theta \sin \theta], \quad (A.2)
\]

\[
H_{12} = \frac{\lambda}{Q} \left\{ \tilde{\gamma} \cos \theta \sin \theta / p \right\} 
+ p[(3B' - B'') \sin^2 \theta + (3B + B'') \cos \theta \sin \theta] 
- 2p[3B \cos \theta \cos \theta + B' \cos^2 \theta], \quad (A.3)
\]

\[
H_{21} = \frac{\lambda}{Q} \left\{ \tilde{\gamma} \cos \theta \sin \theta / p \right\} 
- p[(3B' - B'') \cos^2 \theta - (3B + B'') \cos \theta \sin \theta] 
- 2p[3B \cos \theta \sin \theta - B' \cos^2 \theta], \quad (A.4)
\]

\[
H_{22} = \frac{\lambda}{Q} \left\{ \tilde{\gamma} \sin^2 \theta / p \right\} 
- p[(3B' - B'') \sin \theta \cos \theta - (3B + B'') \cos^2 \theta] 
+ 2p[3B \cos^2 \theta - B' \cos \theta \sin \theta], \quad (A.5)
\]

where

\[
Q = 6B\tilde{\gamma} + p^2[3B(3B + B'') - B'(3B' - B'')], \quad (A.6)
\]

and

\[
B' = \partial B / \partial \theta, \quad B'' = \partial^2 B / \partial \theta^2. \quad (A.7)
\]

Here, we have omitted higher-order terms with respect to \(p = |p|\). From Eq. (A.2), we have \(\partial^2 z/\partial x^2|_{y=y_c(0)} = (\Delta x)^{-1/2}/(2\sqrt{3B(0)})\), with \(p\) being given by Eq. (4.8); and from Eq. (A.5), we have \(\partial^2 z/\partial y^2|_{x=x_c(0)} = 2\Delta y/\sqrt{6B(0)\tilde{\gamma}}\), with \(\theta\) and \(p\) being given by Eqs. (4.11) and (4.12), respectively.

In the \(p \to 0\) limit, therefore, the Gaussian curvature \(K\) of the curved region is obtained as

\[
K = \det(H_{ij}) = \frac{\lambda^2}{6B(\tilde{\gamma})}, \quad (A.8)
\]

Because \(B(\theta) = \pi^2(k_BT)^2/(6\tilde{\gamma}(\theta))\), \(K\) becomes \(\pi^2(k_BT)^2\lambda^2\), which does not depend on \(\theta\).
Appendix B

Geometrical Derivation of the Universal Value of the Shape Exponent

We have another simple geometrical derivation of (4.14) as follows. Very near the point $P$, we take a different point $Q$ on the facet contour (Fig. 15). Along the $x'$-direction chosen normal to the facet contour at $Q$, the ECS profile has the form (4.9) with $B(0)$ replaced by $B(\theta)$, where $\theta (|\theta| \ll 1)$ is the tangent angle (relative to the $y$ axis at $P$) of the facet contour at $Q$. Note that the facet contour near $P$ is approximately a part of a circle whose radius is the curvature radius $R$, which is proportional to the step stiffness $\tilde{\gamma}(0)$. For the normalized ECS, we have $R = \tilde{\gamma}(0)$, and hence, by an elementary geometrical identity, we can relate $\Delta x'$ (the distance along the $x'$ direction) to $\Delta y$ as

$$\Delta x' = \frac{(\Delta y)^2}{2R} = \frac{(\Delta y)^2}{2\tilde{\gamma}(0)}.$$  \hspace{1cm} \text{(B.1)}$$

Replacing this $\Delta x'$ with $\Delta x$ in (4.9), we reproduce (4.14). [We can set $B(\theta) \approx B(0)$, for our purpose.]

Appendix C

Critical Amplitudes of the Profile Near the Facet Edge

Let us discuss the “critical amplitudes” of the profiles. In the derivation of the universal Gaussian curvature jump at the facet edge, the universal relation Eq. (4.15), which holds for any system (with only short-range inter-step interactions), is essential. This relation was originally derived in the coarse-grained TSK picture of the vicinal surface, and it has been confirmed in several ways. For example, an exact calculation with the BCSOS model has been used to verify (4.15) for arbitrary $\theta$. Using (4.15), we obtain a universal relation between the amplitudes of the normal and tangential profiles as follows. By $A_x(\theta)$ and $A_y(\theta)$ we denote the amplitudes of the ECS profiles, namely,

$$z \sim \begin{cases} A_x(\theta)(\Delta x)^{3/2}, & \text{(normal direction)} \\ A_y(\theta)(\Delta y)^{3}. & \text{(tangential direction)} \end{cases} \hspace{1cm} \text{(C.1)}$$

Restoring the scale factor $\lambda$ in (3.9), we have from (4.9), (4.14) and (4.15),

$$[A_x^2(\theta)A_y(\theta)]^{1/3} = \lambda \frac{2}{3\pi k_B T}, \hspace{1cm} \text{(C.2)}$$
which means that at a fixed temperature, the quantity \((A_x^2 A_y)^{1/3}\) is constant along the facet contour. The scale factor \(\lambda\) can be determined, for example, from the measurable ratio \(\kappa/\sigma(\theta)^2 \propto \lambda/(k_B T)\), where \(\kappa\) is the curvature of the facet contour and \(\sigma\) is the scaled fluctuation width of a single step.

We finally give a brief comment on the effect of the long-range inter-step interaction (\(\sim 1/r^2\), with \(r\) being the inter-step distance), which has its origin mainly in the elastic deformation, and is important in the investigation of real crystal surfaces. It is known that inclusion of a \(g/r^2\) interaction with positive coupling constant \(g\) does not modify the GMPT-type form of expansion, but merely renormalizes the coefficient \(B\). The explicit form of the renormalized \(B\) is also known.

Hence, the exponent \(\theta_y = 3\) is not changed by the \(g/r^2\) interaction. Then, because \(\gamma(\theta)\) is a quantity associated with a single isolated step and is not affected by the \(g/r^2\) interaction, the relation between \(\gamma\) and the renormalized \(B\) should be modified. If \(g\) is independent of \(\theta\), the mean running direction of steps, then the universal relation \((C.2)\) still holds in a modified form. However, if \(g\) depends on \(\theta\), \(A_x\) and \(A_y\) will no longer be universally related to each other. In this case, \((C.2)\) may provide a way to determine the \(\theta\) dependence of \(g\) experimentally, by measuring the ratio \([A_x^2(\theta) A_y(\theta)]^{1/3}/[A_x^2(0) A_y(0)]^{1/3}\).

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