Faceting Diagram for Macrosteps at Equilibrium: Tensor Network Calculations

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When faceted macrosteps are formed due to discontinuous surface tension [1], how are the faceted macrosteps formed depending on the temperatures or the surface slope? To study this, we calculated surface free energies numerically for a lattice model for an inclined crystal surface at equilibrium [2,3] using the product-wave-function renormalization group (PWFRG) method [4] which is an extension of the tensor network method [5]. The calculated model was the restricted solid-on-solid model with point-contact-type step-step attractions (p-RSOS model) [1-3], where the step-step attractive energy ε_2 was assumed to be on energy gain forming bond from dangling bonds at the edges of adjacent steps. It should be noted that the model is a coarse-grained one relative to the model for the quantum mechanical calculations [6] and it is a more microscopic model than the one for the phase field theory [7].

We obtained faceting diagrams for the two-surface coexistence corresponding to the connectivity of the surface tension [2,3]. We also obtained a spinodal line for a homogeneously stepped surface as a metastable surface [2]. Comparing our results with the phase diagram for Si (113) + (114) surfaces [8], we estimated $\varepsilon_2 = 123$ meV approximately.

It should be noted that the slope dependence of the two-surface coexistent line cannot be obtained by the terrace-step-kink (TSK) model with point-contact-type step-step attraction. The excited structures on the terrace such as adatoms, ad-holes, and islands are important. Therefore, we used the PWFRG method for calculations of surface free energy on the RSOS model.

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