Faceted-Rough Surface in the Non-Equilibrium Steady State Near Equilibrium

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Are growing surfaces always rough? In this presentation, we show how step-assembling/disassembling affects thermodynamic roughness based on the recently found *faceted-rough surface* near equilibrium using the Monte Carlo method [1]. We focus on step assembling/disassembling and roughness on terrace surfaces. The model we adopted was a restricted solid-on-solid (RSOS) model with a point-contact-type step-step attraction caused by quantum mechanics [2]. Due to the step-step attraction, the step assembles at low temperatures at equilibrium [3,4]. At the same time, the surface free energy becomes discontinuous. The faceted macrosteps with (001) terrace and (111) side surfaces are formed as the result of the discontinuous surface tension. It should be noted that the model is a coarse-grained one relative to the model for the quantum mechanical calculations [5] and it is a more microscopic model than the one for the phase field theory [6].

We calculated the surface width of the inclined surface with the slope $p = 0.530$ using the Monte Carlo method changing system size L [1]. We confirmed that the (001) terrace and (111) side surfaces of the macrostep are atomically and thermodynamically smooth at equilibrium. In the non-equilibrium steady growth, the surface grows in the two-dimensional (2D) nucleation process at the edge of the faceted macrosteps. We found that the growing surface with a single nucleation process is also atomically and thermodynamically smooth. However, the surface becomes thermodynamically rough with the roughness exponents $\alpha = 0.60$ when the surface crosses over to the 2D poly-nucleation growth process at the edge of the macrosteps (the faceted-rough surface) [1]. Here, we denote the crossover point of the driving force for crystal growth $\Delta\mu_c$.

We also calculated the surface growth velocity V. For $\Delta\mu < \Delta\mu_c$, V is nearly zero where the surface grows intermittently by the 2D single nucleation process; for $\Delta\mu_c < \Delta\mu$, the surface grows continuously with substantially smaller velocity [7-9] than that of the inclined surface without macrosteps; this provides a new scenario for strong anisotropy in growth velocity.

References

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