ファセット化したマクロステップの平均高さ：反応（界面）律速定常成長/溶解

Mean Height of the Self-Assembled Faceted Macrosteps: Steady Crystal Growth/Dissolution in a Reaction- (Interface-) Limited Process

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Faceted macrosteps are considered to play critical roles in some reaction- (interface-) limited processes of crystal growth/dissolution [1]. For the diffusion-limited crystal growth, step dynamics of macrosteps or bunched steps with rough side surfaces has been studied theoretically and experimentally [2,3]. Whereas, for the reaction-limited crystal growth/dissolution, the step dynamics of macrosteps has not yet been studied sufficiently.

In this paper, the step dynamics of faceted macrosteps in a reaction- (interface-) limited crystal growth/dissolution is studied theoretically by using a Monte Carlo method for the non-conserved systems. The microscopic model for this Monte Carlo study is the restricted solid-on-solid model with a point-contact step-step attraction (p-RSOS model) [4]. Here, the “restricted” means the height difference between the nearest neighbor sites is restricted to {0, ±1}. The step-step attraction is assumed to be the energy gain ε_{int} by forming a bond between the neighboring steps at the meeting point. The eminent point of this p-RSOS model is that the reliable surface tension (surface free energy per unit normal area) can be calculated at equilibrium by using the density-matrix renormalization-group (DMRG) method [5]. The polar graph of the surface tension (the Wulff figure) calculated by the DMRG method is shown in Fig. 1 [6]. A faceted macrostep is self-organizing at equilibrium because of the discontinuous surface tension resulting from the microscopic step-step attraction [6].

In the non-equilibrium steady state, we found that the height of the macrostep decreases as the driving force of dissolution increases [7]. In the step-faceting zone (Fig. 1 (a)), elementary steps detach from the faceted macrostep by way of the two-dimensional (2D) nucleation at the upper edge of the faceted macrostep on the (001) and the (111) surfaces. Near equilibrium, since the kink densities of the (001) and the (111) surfaces are few, the faceted surfaces cannot move. For the large driving force, the vicinal surface roughens kinetically.

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Fig. 1 Cross section of the Wulff figure and the equilibrium crystal shape (ECS). Thin solid lines: ECS. Thick solid lines and filled squares: polar graph of surface tension. (a) $k_BT/\varepsilon = 0.4$. (b) $k_BT/\varepsilon = 0.63$. Light thin solid lines: polar graph of surface tension for metastable surfaces. (c) $k_BT/\varepsilon = 0.75$. (d) $k_BT/\varepsilon = 0.4$. The original RSOS model. The figures are taken from Ref. [6].

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