Japan Geoscience Union Meeting 2015
(May 24th - 28th at Makuhari, Chiba, Japan)

MIS31-06 Room:102A Time:May 27 10:30-10:45

Numerical simulation of step dynamics: Quantitative formulation based on a phase-field method

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Step dynamics on a crystal surface is one of the fundamental processes of crystal growth. Growth units such as atoms and molecules in the ambient phase are incorporated into kink sites at the step front, and the step then spreads along the crystal surface, resulting in the growth of the crystal in the vertical direction (layer-by-layer growth mechanism). Therefore, the physics of supply and advancement of steps should be clarified for understanding the crystal growth mechanism.

In 1949 a spiral growth mechanism was proposed to explain non-negligible growth of crystals at low supersaturation [1]. If a screw dislocation emerges normally at the crystal surface, it acts as an eternal step source and forms a spiral hillock with the dislocation outcrop as the top. The normal growth rate is given by an analytic formula as a function of supersaturation [2,3]. A formula giving the hillock slope versus supersaturation plus the measurement of the slope as a function of supersaturation allows us to determine the free surface energy of the step riser and the Burgers vector of the step sources [4,5]. However, these analytic formulas do not describe the dynamics of individual steps. Actual growing crystal surface shows complex step behaviors, for example, emergence of a closed-loop step between two dislocations with opposite signs, and formation of new step islands due to two-dimensional nucleation [6]. In order to investigate the effect of the complex step behaviors on the crystal growth, an alternative method that can treat the dynamics of numerous steps simultaneously is required.

In this study, we proposed a new numerical scheme to calculate the dynamics of numerous steps quantitatively based on a phase-field (PF) method. The PF method has been developed as a numerical technique for simulating the step dynamics on crystal surface [7]. In this method, two-dimensional height profile on the crystal surface is expressed by an order parameter termed *phase*, which takes a constant value between steps (terrace) and bridges between two different-height terraces continuously within a finite width. We newly defined a free energy functional including a supersaturation term explicitly and derived a governing equation for the phase field (PF equation) based on the minimum free energy principle. We also formulated the PF equation so that the advancing rate of a straight step corresponds to that determined by the direct integration hypothesis (exact solution) [3] at a small supersaturation limit. We applied this scheme to some step dynamics problems to check the validity. We confirmed that the advancing rate of a straight step could be calculated accurately with optimized computational parameters. We examined the growth and dissolution of a two-dimensional island in supersaturation condition and found that the time evolution of its radius agrees with the analytic solution including the Gibbs-Thomson effect. We also introduced screw dislocations according to [7] to calculate the normal growth rate of the spiral growth mechanism. Our numerical results agreed with the analytic formulas [2,3] in various cases: a single dislocation, a pair of dislocations with opposite/like signs, and an array of dislocations with equal interval.

Note that our simple formulation requires only a single parabolic partial differential equation to be solved numerically. Our scheme would provide a new approach for the study of crystal growth.

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Keywords: Crystal growth, Step dynamics, Numerical simulation, Phase field method