

Models for Calculating Composition of Alloy in Liquid Phase Epitaxy Considering Forced-convection

Hiomoto Susawa

Summary

Liquid Phase Epitaxy is a crystal growth on a substrate from liquid solution, which is a melt in this paper. Before growth, a melt is separated from a substrate and supercooled. When growth starts, the melt moves to the substrate. This induces flow in the melt. This paper considers the influence of flow on the composition of solid phase, reviews previous simulation models and introduces a new model. A one-dimensional model explained an experimental result and a major behavior of solid compositional variation. A semi-two-dimensional (semi-2-D) model dealt with transport in the melt as 2-D but substituted the values at the mid point of growth interfaces for ones at the all points on the interface and showed eddies' 2-D effects. At present, a full-2-D model solves all the boundary conditions without the substitution. Navier-Stokes equations describe the flow and are solved with Computational Fluid Dynamics. These models target to replace experiments fabricating electronic devices. Then set the tolerance of solid composition. Diffusion equations of solutes in the melt, which include the solved velocity of flow, are solved by finite difference method. The determination of mesh size needs systematic approach to satisfy the above tolerance. The composition on growth interface depends on supplies of solutes in the melt through diffusion, satisfying the equilibrium state on the interface. The solid and liquid solutions are approximated to regular solution. Full-2-D model describes that the compositions vary at each place on the growth interface. As a result, the solid composition varies larger than the semi-2-D model by 6 times the above tolerance. The semi-2-D model predicts the outline and reduces calculation cost. CPU time was measured for each model. These modes can be selected, considering cost performance. Treated phenomenon is fundamental and generalized. The shown methods will be applied to likely industrial processes or other fields.

