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IMPLICIT NUMERICAL ALGORITHM FOR SOLUTION OF PHASE TRANSITION PROBLEMS IN MULTI-COMPONENT ALLOYS

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The report presents the new numerical procedure for computer simulation of crystallization problems. A solid-liquid diffusion model for equilibrium multi-component alloy solidification is developed [1]. One-dimensional model allows to simulate diffusion limited crystal growth that is favorable in many cases from material quality point of view. The developed model is based on diffusion equations for species concentrations in solid phase and melt. Accounting for diffusion in solid phase allows to set up self-consistent mathematical model that provides the possibility for full scale computer simulation of growth and dissolution processes. In solidification of multi-component alloys concentrations of all species and crystal growth rate are strongly coupled at the interface by mass balance equations and phase diagram. This feature is crucial for designing reliable numerical procedure.

The handle equation of solid-liquid interface the moving boundary problem is mapped to new coordinate system where the interface is fixed. Conservative and implicit finite difference scheme is obtained in new coordinate system with control volume technique [2]. Equation coefficients corresponding to coordinate system transformation, that is determined by crystal growth rate, are approximated in implicit way. Corresponding set of nonlinear equations is solved by Newton method for unknown vector, which components are concentrations of all species and crystal growth rate. Linearized set of equations is solved with the help of the specially designed sweep method [3]. Thus, conservative fully implicit scheme is realized with simultaneous determination of concentration distribution and interface position. The proposed numerical procedure appears to be unconditionally stable.

The report provides a comparison of new algorithm with traditional ones, where concentration distribution and interface position (growth rate) are determined consequently. The developed algorithm is applied to numerical study of liquid phase epitaxy of ternary alloys. The computer simulations is done for real phase diagram and experimentally used growth conditions.

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