3D computer simulation of convective instability in the multicomponent solution

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The paper presents the numerical study of natural convection in solidification of ternary nondilute solution. The problem arises in computer simulation of liquid phase epitaxy (LPE), classified as a solution growth process. In distinction to solidification of pure materials or dilute alloys phase transition temperature in epitaxial growth depends on the composition of the liquid and solid phases.

The process is described by 3D time-dependent Navie-Stockes and mass transport equations. The solution is supposed to be incompressible and Boussinesq approximation is adopted. The interface conditions consist of the mass balance between the transported and incorporated solute species and phase diagram representing the equilibrium between the solution and growing layer.

The governing equations are discretized at staggered grid using control-volume method. Approximation of convective terms ensure kinetic energy conservation and mass balance for dissolved components. The scheme is implicit, has second order in space, first in time. Navier-Stokes equations and mass transfer equations are solved successively at each time level. To determine velocity and pressure fields we follow predictor-corrector procedure. The calculated velocity field is substituted into the mass transfer equations, that are solved with coupled algorithm [1], extended to 3D case.

Full scale computer simulation for actual materials under reasonable operating conditions has been done for Rayleight number varying in the range $1.1 \cdot 10^3 < Ra < 1.1 \cdot 10^5$, $Sc_i = 50$.

The onset of convective motion is observed at $Ra = 1100$. The calculations show a transition from initial non-regular flow pattern to hexagonal planform. This finite amplitude subcritical convective motion has been predicted by theoretical analysis [2] and evolves due to nonlinear concentration profile. The flow direction at the center of the cells depends on the profile curvature sign. The run duration is approximately 25 diffusion times.

In the range $1.1 \cdot 10^3 < Ra < 1.4 \cdot 10^4$ a regular cellular convection pattern is obtained. At Rayleight number of $1.4 \cdot 10^4 \div 3 \cdot 10^4$ the transition to skewed-varicose and knot instability is registered [3]. The mean convective structure size increases with Ra while $Ra < 3 \cdot 10^4$. Above $Ra = 3 \cdot 10^4$ chaotic cellular small-scale convection is detected. The mean cell size at $Ra = 3.5 \cdot 10^4$ several times less then at $Ra = 1.8 \cdot 10^4$.

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Concentration field (view from the top)

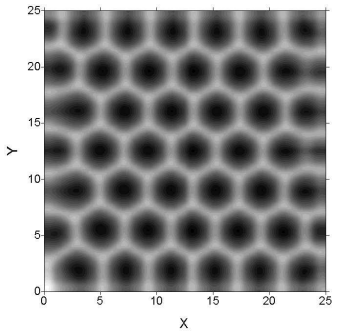

Figure 1: $Ra = 1 \cdot 10^3$

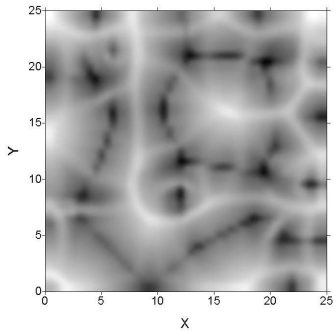

Figure 2: $Ra = 2.5 \cdot 10^3$

References

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