

Deterministic and Probabilistic models of micro-structure formation

– a primary investigation

Project Proposal

Introduction

Solid-liquid phase transition has been under investigation for many years. However, the complex nature of solid-liquid phase change requires a multi-scale approach. On the one hand, the formation of nuclei in an undercooled melt is full of molecular randomness; on the other hand, the growth of crystals and the eventual habit they construct are highly sensitive to and dependent on shapes of the initial nuclei. In this sense, even the tiniest differences in the atomic arrangements and the smallest fluctuations in the flow and temperature field in the melt can cause dramatic distinctions in the growth process that follows. Therefore, a multi-scale combined deterministic and probabilistic model seems necessary to fully resolve the mysteries on solid-liquid phase transition.

Tasks

1. Read the literature in the reference and understand the meanings and connections between the deterministic and probabilistic models
2. Understand how to connect these models
3. Think of a way to implement your idea via programming

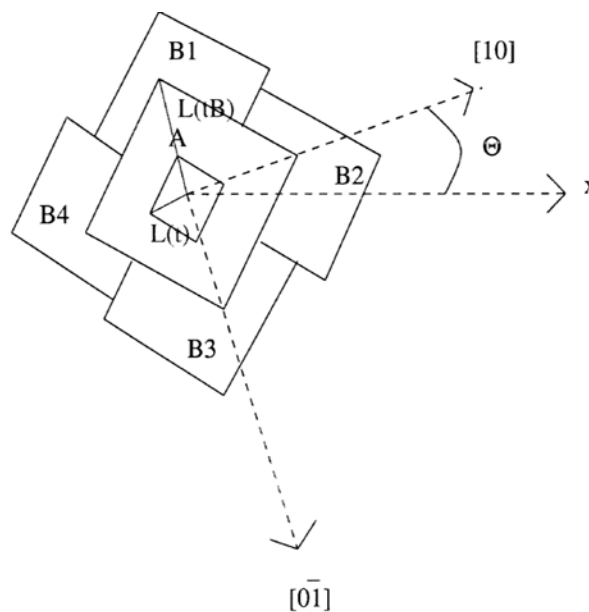


Figure. Model of the grain growth in the Rappaz model

Reference

- [1] H. Rafii-Tabar and A. Chirazi, *Physics Reports* 365 (2002) 145–249

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