

Contents

| | |
|------------------------------------|----------|
| Contents | a |
| 1 Introduction | 1 |
| 1.1 General introduction | 1 |
| 1.2 Motivation | 2 |
| Bibliography | 3 |



Chapter 1

Introduction

1.1 General introduction

This work aims to bring insight into the effect of anisotropy in interface energy for the texture formation during deposition of polycrystals. Specifically it focuses on the effect of anisotropy in interface energy on orientation selection during repeated nucleation in the film growth. To the best knowledge of the author, this relation has not yet been investigated.

Major part of the thesis concerns technical development and validation of multi-phase field models incorporating anisotropic interface energy. Own solver for the partial differential equations composing the model was written in MATLAB, hence there was high need for validation of every aspect of the programme. Multiple model variants were developed and methodology modified several times in order to solve various difficulties emerging due to inherent limitations of the models. Mutual comparison of the developed models was an additional motivation to develop some benchmarking strategies.

The first publication of the author quantitatively compared three multi-phase field models incorporating inclination-dependent interface energy and kinetic coefficient. Two model-independent benchmark problems we developed by the author for the purpose. One assessed the quality of match to Wulff shapes and the shrinkage rate of the shape and the second did the same but in a specific combination of the anisotropy in interface energy and kinetic coefficient, validating thus both features of the model at once.

Because the multi-phase field models are known to reproduce motion of the

interfaces driven by curvature driving force, their typical application is grain growth (disregarding the possibility to include other physics in the model). From the perspective of model development, it is critical to assure correct representation of the force balance in the triple junctions. However, this is a non-trivial requirement due to numerical artifacts called ghost phases, which are in general hard to avoid in multi-phase field models.

Development of benchmark problems allowing quantification of multi-phase field model performance in triple junctions was thus recognized as highly relevant for the community. A collaboration was initiated with another scientific group at Karlsruhe Institute of Technology, Karlsruhe, Germany, which had expertise in a different type of multi-phase field models. In another two benchmarks focusing on triple junctions, a wide group of multi-phase field models was compared and a publication was produced, co-authored by the author.

The purpose of the herein developed models was to identify equilibrium stable shapes of heterogeneous nuclei with inclination-dependent interface energy as function of the nucleus and substrate crystallographic orientation. This knowledge can be used to derive the anisotropy in nucleation probability as function of the crystallographic orientations. Even though the multi-phase-field framework was developed enough to provide the results, the geometrical problem has an analytical solution.

Knowledge of the analytic solution allowed to implement a much simpler and more efficient algorithm, providing deeper and more reliable insights. So-called shape factor-orientation maps were constructed with high resolution and were used as input in a Monte Carlo simulation of growing polycrystal to demonstrate how the nucleation with anisotropic interface energy may affect the course of texture evolution. New modes of texture evolution were identified and the insight was used to qualitatively explain an experimentally observed peculiar texture evolution in electrodeposited nickel. The latter findings were published in a third paper the author was involved in during his PhD research (as main author).

1.2 Motivation

Bibliography