# SUMMARY OF Ph.D. DISSERTATION


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Title

Multiscale Modeling and Simulation of Crystal Plasticity Based on Dislocation Patterning and Accumulation of GN Dislocation


**Abstract**

Elementary processes of plastic deformation and work-hardening of a crystal are known to be dislocation motions and accumulations, respectively. Recently, studies on theory of multiscale plasticity incorporating dislocation information into a hardening law of a crystal have actively been done by many researchers. While, ultrafine-grained metals (UFGM) have attracted interest as high-strength materials. It is expected in the field of material textures control that a microscopic mechanism of production process for UFGM is numerically predicted by synthesizing knowledge obtained from computational materials science and computational solid mechanics. However, such a study has never been reported. In this thesis, aiming at a prediction of production process of UFGM, reaction-diffusion equations describing the self-organization of collective dislocations is derived, and the geometrically necessary (GN) crystal defects are newly defined on the basis of the differential geometry of dislocation field. A multiscale crystal plasticity model is developed, that enables to exchange the information of dislocation field and deformation field. Multiscale simulations based on this model are carried out and a process of fine-graining is computationally reproduced under a severe strain condition.

Chapter 1 is an introduction summarizing a background of this study and problems of previous studies.

Chapter 2 devotes kinematics used in this thesis. Two kinds of densities of GN crystal defects, i.e., GN dislocation density and GN incompatibility corresponding to isolated dislocation and dislocation pairs, respectively, are newly defined so that these quantities are consistent with the framework of crystal plasticity theory. Through some geometrical considerations on the GN crystal defects, a model is proposed that expresses a dynamic recovery of dislocation due to an annihilation of dislocation pair.

In chapter 3, internal variables are determined as arguments of total free energy, and balance equations are derived by defining thermodynamic forces conjugate to the arguments. An entropy inequality is obtained from the second law of thermodynamics taking account of an entropy flux of diffusion that means a dislocation mobility contributing to the self-organization of dislocation.

In chapter 4, constitutive equations are thermodynamically developed by decomposing the constitutive quantities into conservative and dissipative parts so that these parts satisfy the principle of increase of entropy. Reaction-diffusion equations governing dislocation patterns such as cell structure and subgrain are derived by applying the constitutive equations of dislocation density flux to the balance equations obtained in chapter 3. A generation criterion of Turing bifurcation causing spatially inhomogeneous structures and a spontaneous length scale of dislocation structure are determined by a linear stability analysis for the reaction-diffusion equations.

In chapter 5, a general method is shown for introducing the information of dislocation density into the hardening modulus of a crystal. An elastoviscoplastic constitutive equation for crystal plasticity is derived by use of the anisotropic elastic constitutive equation obtained in chapter 4. Stress effect coefficients are modeled by reflecting stress information on the dislocation field. A dislocation-crystal plasticity FEM is explained in detail as a preliminary to numerical analyses in chapters 7 and 8.

In chapter 6, Two-dimensional FD simulation is conducted using the reaction-diffusion equations. Each rate coefficient of reaction-diffusion equations and spontaneous length scale are quantitatively investigated on the basis of calculated dislocation patterns.

Chapter 7 devotes a dislocation-crystal plasticity simulation using the stress effect coefficient model mentioned in the previous chapter and introducing the immobile dislocation density obtained from the reaction-diffusion equations into the hardening modulus of a crystal as information of dislocation field. A dislocation patterning simulation and a deformation analysis for single crystal of Al are simultaneously computed with FDM for the former and FEM for the latter. It is shown that the numerical results on formation of cell structure and subgrain are suitable for the experimental dislocation patterns observed in stage II and stage III on the basis of visualized distributions of accumulated dislocation density, slip and crystal orientation.

In chapter 8, a dislocation-crystal plasticity FE analysis using the GN crystal defects for the hardening modulus of a crystal is performed for a polycrystal of Al at a severe compression strain. It is discussed that the present dynamic recovery model is valid as well as the dislocation mean free path model depending on dislocation density. The generation process of GN boundaries induced in a grain is reproduced and it is clarified that an initial grain is separated into plural fine grains by the GN boundaries.

Chapter 9 describes conclusions of this thesis.