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Dislocation microstructures and strain-gradient plasticity with one active slip plane

Sergio Conti [a,*], Adriana Garroni [b], Stefan Müller [a]

[a] Institut für Angewandte Mathematik, Universität Bonn, 53115 Bonn, Germany
[b] Dipartimento di Matematica, Sapienza, Università di Roma, 00185 Roma, Italy

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ABSTRACT

We study dislocation networks in the plane using the vectorial phase-field model introduced by Ortiz and coworkers, in the limit of small lattice spacing. We show that, in a scaling regime where the total length of the dislocations is large, the phase field model reduces to a simpler model of the strain-gradient type. The limiting model contains a term describing the three-dimensional elastic energy and a strain-gradient term describing the energy of the geometrically necessary dislocations, characterized by the tangential gradient of the slip. The energy density appearing in the strain-gradient term is determined by the solution of a cell problem, which depends on the line tension energy of dislocations. In the case of cubic crystals with isotropic elasticity our model shows that complex microstructures may form in which dislocations with different Burgers vector and orientation react with each other to reduce the total self-energy.

1. Introduction

Michael Ortiz and coworkers (Ortiz, 1999; Koslowski et al., 2002; Koslowski and Ortiz, 2004) proposed the use of a vector-valued phase field as a device for describing complex dislocation arrangements. Their model permits to study situations in which multiple slip systems are active, as long as the activity is limited to a single slip plane. It incorporates both a local Peierls interplanar nonconvex potential, which characterizes the discrete nature of slip, and long-range elastic energy. Numerical simulations permitted to identify stable dislocation structures in finite twist boundaries (Koslowski and Ortiz, 2004). The optimal structures obtained from the simulations exhibit a pattern containing regular square or hexagonal dislocation networks, separated by complex dislocation pile-ups.

The classical analysis of dislocations is based on regularized continuum models, see Hirth and Lothe (1968) and Hull and Bacon (2011). The need for a regularization arises from the $1/r$-divergence of the strain close to the singularity, and is often implemented either by excluding a small volume around the core or by smoothing the singularity, in both cases on a length scale of the order of the lattice spacing ε. In reality, in a discrete lattice there is no singularity, and indeed the mathematical analysis of dislocation models has shown that the regularization in continuum models plays the same role as the lattice spacing in discrete ones. The Ortiz phase-field model, as well as the Nabarro–Peierls model, can be seen as a different way of regularizing linear elasticity. The Nabarro–Peierls model is often understood to be a one-dimensional model for straight dislocations, but natural extensions to curved dislocations have permitted to study the energetics of dislocation loops, see for example Xu and Ortiz (1993), Xu and Argon (2000), and Xiang et al. (2008).

* Corresponding author.
E-mail address: sergio.conti@uni-bonn.de (S. Conti).

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The mathematical analysis of the phase-field model highlights the occurrence of microstructures over many different length scales. Focusing on the regime where the leading-order contribution to the total energy is given by the dislocation line tension, a number of mathematical papers rigorously characterized the asymptotics of the model within the framework of Γ-convergence. This was started in Garroni and Müller (2005, 2006) for the scalar case in which all dislocations have the same Burgers vector, then extended in Cacace and Garroni (2009) and Conti et al. (2011) to the vectorial situation with multiple slip, and in Conti and Gladbach (2015) to dislocations localized to two parallel planes. One key result is that straight dislocations with certain Burgers vectors and orientations may spontaneously decompose into several parallel dislocations, and in some cases a zig-zag structure is optimal, see Cacace and Garroni (2009), Conti et al. (2015a), and Conti and Gladbach (2015). These mathematical results gave a rigorous foundation to the classical Frank's rule for dislocation reaction (Hirth and Lothe, 1968; Hull and Bacon, 2011).

A fully three-dimensional discrete model for dislocations and plasticity was proposed by Ariza and Ortiz (2005), see also Ramasubramaniam et al. (2007). Their model offers a general framework for dislocations in a lattice, and is amenable to a simple analysis of the continuum limit in situations where Fourier methods are appropriate. In the line-tension scaling, more complex techniques are however necessary to pass to the continuum limit. A rigorous derivation of a line-tension model from linear elasticity with core regularization was given in Conti et al. (2015b), an extension to a discrete model of the Ariza–Ortiz type will appear in Conti et al. (2016a). Also in this case, relaxation of straight dislocations may be observed, leading to a line-tension energy which may be smaller (Conti et al., 2015a,b) than the one predicted by the classical prelogarithmic factor based on an *ad hoc* generalized plane-strain *ansatz* (Barnett and Swanger, 1971; Rice, 1985).

Energy relaxation by formation of microstructure may be even more relevant in a situation in which one studies the collective behavior of many dislocations. Precisely, one considers a situation in which the total length of the dislocation lines diverges, and one observes a continuous, macroscopic distribution of dislocations. Whereas one can estimate the energy of an average dislocation density by adding the energies of the individual dislocations, interaction and relaxation effects may significantly alter the picture. This is a well-known effect in the phenomenological study of low-angle grain boundaries, see for example Hirth and Lothe (1968) and Gottstein (2014). We give here a general formulation and a mathematically rigorous treatment. In particular, we show in Section 4 that in specific geometries dislocations with different orientations and Burgers vectors may interact, leading in some cases to complex zig-zag patterns. Geometrically, the total (tensorial) density of dislocations corresponds to the total incompatibility of the elastic strain field, and therefore to its (distributional) curl. For this reason, the energy of a dislocation density plays a fundamental role in the regularization of models of crystal plasticity, leading to the so-called strain-gradient plasticity models (Fleck and Hutchinson, 1993, 2001; Nix and Gao, 1998; Bassani, 2001; Conti and Ortiz, 2005; Kuroda and Tvergaard, 2008; Fokoua et al., 2014). Indeed, the presence of large latent hardening renders the variational problem of crystal plasticity, within the deformation theory, nonconvex, leading to lack of existence of minimizers due to the spontaneous formation of fine structure, such as slip bands (Aubry and Ortiz, 2003; Ortiz and Repetto, 1999), which can again be treated by the theory of relaxation (Conti and Ortiz, 2005; Conti and Theil, 2005; Conti et al., 2013; Anguige and Dondl, 2014). The phase-field model by Ortiz and coworkers that we study here was related to strain gradient plasticity in Hunter and Koslowski (2008), where in particular the parameters of continuum strain-gradient plasticity approach were derived from the phase-field dislocation model. The corresponding process for the forces is the derivation of a continuum approximation for the Peach–Kohler force, as derived in Xiang (2009) and Zhu and Xiang (2014). We remark that in all these works the *relaxation* of the dislocation structures, which naturally arises if a mathematically rigorous variational limiting procedure is attempted, is not considered.

Strain-gradient plasticity models can be rigorously derived from discrete models, or regularized semidiscrete models, using Γ-convergence with a choice of the scaling of the energy which balances the contributions of the elastic field and of the dislocation core energies. This was performed for the first time for point dislocations in the plane by Garroni et al. (2010) in a geometrically linear setting with a core regularization approach, and by Müller et al. (2014, 2015) with a geometrically nonlinear formulation. Both results rely on a well-separation assumption, which permits to locally estimate the self-energy of each individual dislocation. The assumption of point dislocations in the plane corresponds to an array of straight parallel dislocations in three dimensions.

In this work, we derive a strain-gradient model for a density of line dislocations in the plane. Our starting point is the vectorial phase-field model developed by Ortiz and coworkers. Our key result is that the energy can be approximated by the sum of two terms, given by the long-range elastic interaction and the self-energy of the dislocation density, see (5.8) below. The self-energy itself is determined by solving a cell problem, which corresponds to selecting the energy of the optimal dislocation structure among all those with the same average dislocation density. In particular, it is in general smaller than the sum of the line-tension energies obtained using individual straight dislocations. We remark that the key ingredient in this relaxation is the anisotropy of the prelogarithmic factor in the energy of a single, straight dislocation. Higher-order interaction effects may further enrich the picture.

We introduce in Section 2 the vectorial phase-field model on a torus that we shall use for the rest of the paper and the relevant scaling regime. The line-tension energy of individual dislocations is discussed in Section 3, and the energy of dislocation structures in Section 4. Finally, in Section 5 we present the full limiting model which contains both elasticity and dislocation self-energy.