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Microscopically derived free energy of dislocations

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ABSTRACT

The dynamics of large amounts of dislocations is the governing mechanism in metal plasticity. The free energy of a continuous dislocation density profile plays a crucial role in the description of the dynamics of dislocations, as free energy derivatives act as the driving forces of dislocation dynamics.

In this contribution, an explicit expression for the free energy of straight and parallel dislocations with different Burgers vectors is derived. The free energy is determined using systematic coarse-graining techniques from statistical mechanics. The starting point of the derivation is the grand-canonical partition function derived in an earlier work, in which we accounted for the finite system size, discrete glide planes and multiple slip systems. In this paper, the explicit free energy functional of the dislocation density is calculated and has, to the best of our knowledge, not been derived before in the present form.

The free energy consists of a mean-field elastic contribution and a local defect energy, that can be split into a statistical and a many-body contribution. These depend on the density of positive and negative dislocations on each slip system separately, instead of GND-based quantities only. Consequently, a crystal plasticity model based on the here obtained free energy, should account for both statistically stored and geometrically necessary dislocations.

1. Introduction

The governing mechanism of metal plasticity is the dynamics of dislocations, which are line-like defects in the crystal structure. Crystals can contain up to 10^9 dislocation lines intersecting a square millimeter. Therefore, the collective behavior of many dislocations together determines the mechanical properties associated with crystal plasticity.

A number of dynamical frameworks have been developed to describe the dynamics of dislocation densities, in which the free energy plays a key role, see e.g. Groma (1997), Gurtin (2000), Gurtin and Anand (2005), Gurtin et al. (2007) and Gurtin (2008, 2010). Moreover, stationary states have been derived from the free energy, see e.g.. Groma et al. (2006), Scardia et al. (2014), and Geers et al. (2013).

To obtain the equilibrium behavior and driving forces for dislocations on a macroscopic scale, it is thus necessary to have a free energy expression that results from coarse-graining the microscopic description of dislocations. Furthermore, a derivation from the microscopic level could help in choosing proper macroscopic variables for a dynamical model.

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In the literature, several attempts have been made to retrieve the free energy of dislocations. First, different phenomenological assumptions are made to match different macroscopic plasticity models, see e.g. Ertürk et al. (2009), Bayley et al. (2007), Svendsen (2002), Klusemann et al. (2012) and Bargmann and Svendsen (2012). These free energy expressions are all local or weakly non-local in terms of the dislocation densities.

Second, straight dislocations were considered as an example of two-dimensional Coulomb particles that interact with a logarithmic interaction potential, see e.g. the work of Kosterlitz an Thouless (Kosterlitz and Thouless, 1973; Nelson, 1978; Nelson and Halperin, 1979), Mizushima (1960), Ninomiya (1978) and Yamamoto and Izuyama (1988). In these papers, the free energy of systems with an homogeneous dislocation density was derived. This system exhibits a dislocation mediated melting transition. Below the critical temperature, dislocations occur in tightly bound pairs, but above this temperature, dislocation pairs tend to unbind, and thereby destroy the long-range order in a two-dimensional crystal. However, the anisotropic character of the dislocation interaction was not taken into account in these works, and the effect of mechanical loading was not considered.

Third, the free energy of dislocations was derived by Groma and coworkers using a mean-field assumption in the coarse-graining (Groma and Balogh, 1999; Groma et al., 2006, 2007). As the physical temperature of the system is almost zero relative to the other characteristic energy scales at hand, a second, phenomenological temperature is introduced to obtain a non-vanishing statistical contribution, which results in screening.

Fourth, the equilibrium dislocation profile of a single slip system of dislocations was determined by means of Γ-convergence of the energy expression, see Scardia et al. (2014), Geers et al. (2013). In this work, it was assumed that the dislocations are arranged in wall structures on equally spaced glide planes and that the system is at zero temperature.

Despite all these efforts, no explicit free energy expression has been proposed yet, that is derived from the microscopic properties of the system, and thus includes the anisotropy of the dislocation interaction, the finite system size and the presence of glide planes, and which is valid in different temperature regimes. The aim of this paper is to obtain such a free energy expression. In this contribution, we limit ourselves to straight dislocations with parallel line orientation.

The free energy is derived by systematically coarse-graining the microscopic description of dislocations as used in Discrete Dislocation Dynamics (DDD) simulations. In an earlier paper (Kooiman et al., 2014), we derived the partition function of dislocations for a grand-canonical ensemble of straight and parallel dislocations. In this contribution, we derive the Helmholtz free energy of dislocations from this by means of a Legendre transform. The obtained free energy contains elastic energy and statistical terms, as found earlier by Groma et al. (2006), but yields also a many-body contribution beyond these mean-field terms. It is, to our best knowledge, for the first time that the free energy was derived by coarse-graining only.

The resulting free energy depends on densities of positive and negative dislocations separately for each slip system. This implies that the defect forces in crystal plasticity models (see e.g. Gurtin, 2008) cannot be determined in terms of GND densities alone.

The paper is organized as follows. In Section 2, we discuss the microscopic and macroscopic descriptions of the system. Then, we briefly outline the derivation of the grand-canonical partition function and perform a Legendre transform to obtain the canonical free energy in Eq. (2.22). In Section 3, we discuss the interpretation and limitations of the obtained free energy expression. In Section 4, three special cases are considered in which the free energy expression simplifies considerably, namely a local density approximation (LDA), the zero temperature limit, and equally spaced glide planes. In Section 5, the connection is made between this work and current dislocation-based crystal plasticity models.

2. Derivation

2.1. Mathematical preliminaries

In this paper, both two-dimensional and three-dimensional position vectors are used. To avoid confusion, the two-dimensional position vector is denoted by $\boldsymbol{s}$ and consists of an x and a y-coordinate. Integration over this vector is denoted by $\int dA$. On the other hand, the three-dimensional position vector is denoted by $\boldsymbol{r}$ and consists of an x, y and z-coordinate. Integration over the 3D position vector is denoted by $\int dV$.

The line direction $\hat{\boldsymbol{\xi}}$ of the straight and parallel dislocations is parallel to the $\hat{z}$-direction, and the position in this direction is denoted by z. Thus, the vector $\boldsymbol{r}$ can be expressed in $\boldsymbol{s}$ and z by $\boldsymbol{r} = \boldsymbol{s} + z\hat{\boldsymbol{\xi}}$, and analogously, the integration over 3D position vectors can be expressed as $\int dV = \int dA \int dz$. See Fig. 1 for a sketch of the coordinate system.

In this work, the cross product on a tensor is interpreted as the cross product on the first index, so the cross product between vector $\boldsymbol{v}$ and second rank tensor $\boldsymbol{A}$ is $(\boldsymbol{v} \times \boldsymbol{A})_{ij} = \epsilon_{ikl} v_k A_{lj}$, where ϵ is the anti-symmetric Levi–Cività tensor. A contraction of a second rank tensor $\boldsymbol{A}$ and a fourth rank tensor B is defined by $(\boldsymbol{A}\colon \mathrm{B})_{kl} = A_{ij} B_{ijkl}$, and the trace of a fourth rank tensor B is $\mathrm{Tr}\big[\mathrm{B}\big] = B_{ijij}$. The symmetric and anti-symmetric parts of a second rank tensor are indicated with a superscript s and a; $(\boldsymbol{A}^{\mathrm{s,a}})_{ij} = (A_{ij} \pm A_{ji})/2$. The $\otimes$-symbol is used to indicate a dyadic product.

In this work, round brackets indicate a function, and square brackets indicate a functional.

Furthermore, Fourier transforms are used multiple times in this contribution. We use the non-unitarian convention here,