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Energy of dislocation networks

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ABSTRACT

It is obtained an expression for energy of a random set of dislocation lines. It is used to determine the characteristics of dislocation ensembles which can appear in continuum theory of dislocations.

1. Introduction

One of the basic problems in modeling of plasticity of metals is an identification of state variables. The problem is not simple, because dislocation networks controlling the process of deformation are extremely complex random sets. Among recent works on this subject note the papers by Zaiser (2015), Hochrainer (2015), Hochrainer (2016), Le (2016), Mohamed, Larson, Tischler, and El-Azab (2015d), Hochrainer, Sandfeld, Zaiser, and Gumbsch (2014), Poh, Peerlings, Geers, and Swaddiwudhipong (2013a), Poh, Peerlings, Geers, and Swaddiwudhipong (2013b), Geers, Peerlings, Peletier, and Scardia (2013), Mesarovic, Baskaran, and Panchenko (2010), Zaiser and Hochrainer (2006), El-Azab (2000), Ghoniem, Tong, and Sun (2000). In this paper, some intrinsic probability characteristics of dislocation networks are introduced, and energy is found in terms of these characteristics from homogenization reasoning. The key role is played by dislocation density correlation tensor. Remarkably, it has a singularity. This simplifies the choice of approximations. A simple approximation of dislocation density correlation tensor is considered. It yields the formula for energy and the corresponding set of macroscopic state variables. An interesting outcome is a confirmation of the phenomenological assumption (Berdichevsky, 2006; 2006a) that averaged dislocation density tensor can enter into continuum theory of dislocations without a small parameter. A consequence is that applications of the theory are much broader than just description of size effects in strain gradient plasticity.

We begin the consideration with a formula for energy of one dislocation line (Section 2), then introduce intrinsic probability characteristics (Section 3), express energy in terms of these characteristics (Section 4), introduce correlation tensor and it's approximations (Section 5), obtain the corresponding relations for energy (Section 6), and discuss an alternative mechanism for dependence of energy on averaged dislocation density tensor in Section 7.

2. Energy of one dislocation loop

Consider homogeneous anisotropic elastic body occupying an unbounded three-dimensional space R_3. Let $\alpha_{ij}(x)$ be dislocation density tensor, Latin indices run through values 1, 2, 3, x denotes points in R_3. Then elastic energy of the body has

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the form (see, e.g. Mura, 1991),

$$E = \int_{R_3}\int_{R_3} \frac{1}{2} H^{mnpq}\left(\frac{x-\tilde{x}}{|x-\tilde{x}|}\right)\frac{1}{|x-\tilde{x}|}\alpha_{pm}(x)\alpha_{qn}(\tilde{x})dV_x dV_{\tilde{x}}. \tag{1}$$

Here dV_x and $dV_{\tilde{x}}$ are volume elements in x and $\tilde{x}$-variables, summation over repeated indices is implied, $H^{mnpq}(\vec{\xi})$ is a tensor defined on unit vectors $\vec{\xi}$ and expressed in terms of Green's tensor. $H^{mnpq}(\vec{\xi})$ are even functions of $\vec{\xi}$. The explicit form of $H^{mnpq}(\vec{\xi})$ is not essential for what follows.

For one dislocation loop Γ with Burgers vector b_i,

$$\alpha_{ij}(x) = b_i t_j\, \delta(\Gamma), \tag{2}$$

t_i is tangent vector to Γ, $\delta(\Gamma)$ delta-function of Γ,

$$\delta(\Gamma) = \int_\Gamma \delta_3(x - r(s))ds,$$

$x = r(s)$ the parametric equations of Γ, s arc length on Γ, $\delta_3(x) = \delta_1(x_1)\delta_1(x_2)\delta_1(x_3)$, x_i are components of x, δ_1 is one-dimensional delta-function. Note that

$$\int_{R_3} \delta(\Gamma)dV_x = |\Gamma|, \tag{3}$$

$|\Gamma|$ being the length of Γ.

Substitution of (2) in (1) yields a diverging integral, and a regularization of (2) is needed. As such we use the following construction: we embed Γ into a tube Γ_a with a circular cross-section of radius a in such a way that Γ passes through the centers of cross-sections, and replace $\delta(\Gamma)$ in (2) by $\chi(\Gamma_a)/\pi a^2$, where $\chi(\Gamma_a)$ is the characteristic function of region Γ_a, i.e. $\chi(\Gamma_a) = 1$ inside of Γ_a and $\chi(\Gamma_a)$ is zero outside of Γ_a. So, we set

$$\alpha_{ij}(x) = b_i t_j\, \chi(\Gamma_a)/\pi a^2, \tag{4}$$

and consider the limit $a \to 0$. Obviously, for $a \to 0$

$$\int_{R_3} \frac{\chi(\Gamma_a)}{\pi a^2} dV = |\Gamma|.$$

Parameter a plays the role of dislocation core radius. It is supposed to be chosen in such a way that elastic energy of the region Γ_a coincides with energy of the dislocation core. Alternative ways of regularization have been reviewed and discussed by Cai, Arsenlis, Weinberger, and Bulatov (2006), see also Lazar and Maugin (2005), Lazar and Po (2014), Aifantis (2009), Po, Lazar, Seif, and Ghoneim (2014).

From (1) and (4)

$$E = \int_{\Gamma_a}\int_{\Gamma_a} \frac{1}{2} H^{mn}\left(\frac{x-\tilde{x}}{|x-\tilde{x}|}\right)\frac{1}{|x-\tilde{x}|} t_m(s)t_n(s')dsds' \frac{d^2X}{\pi}\frac{d^2X'}{\pi}. \tag{5}$$

Here

$$H^{mn} = H^{mnpq} b_p b_q,$$

X^μ are dimensionless Cartesian coordinates in cross-sections chosen in such a way that cross-section is determined by the inequality $X^\mu X_\mu \le 1$. The determinant of the transformation to (s, X)-coordinates is skipped in (5) because it is equal to unity in the limit $a \to 0$.

Various asymptotically equivalent approximations of energy for $a \to 0$ can be used (see Cai et al., 2006). We will employ the following relation[1], which does not seem to have been known,

$$E = \int_\Gamma\int_\Gamma \frac{1}{2} H^{mn}\left(\frac{\vec{r}(s') - \vec{r}(s)}{\left|\vec{r}(s') - \vec{r}(s)\right|}\right)\frac{t_m(s)t_n(s')}{ca + \left|\vec{r}(s') - \vec{r}(s)\right|}dsds' \tag{6}$$

where

$$c = \frac{1}{2}e^{-1/8} = 0.44.$$

Formula (6) follows from (5) and can be derived in the same way as the similar expression for kinetic energy of vortex filament in ideal incompressible fluid (see Berdichevsky, 2008, Berdichevsky, 2009, p. 437–440)[2]. Note that the above-mentioned choice of a making elastic energy of region Γ_a coinciding with energy of dislocation core yields the dependence

[1] In contrast to vectors associated with R_3, like x and $\tilde{x}$ in (5), all vectors associated with dislocation lines are provided by arrow, like $\vec{r}(s)$ and $\vec{r}(s')$ in (6).

[2] Parameter a in dynamics of vortex filaments changes in the course of motion, therefore it was convenient to use a different asymptotically equivalent form of energy when a is kept outside of integrals.