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Dislocation field theory in 2D: Application to graphene

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ABSTRACT

A two-dimensional (2D) dislocation continuum theory is being introduced. The present theory adds elastic rotation, dislocation density, and background stress to the classical energy density of elasticity. This theory contains four material moduli. Two characteristic length scales are defined in terms of the four material moduli. Non-singular solutions of the stresses and elastic distortions of an edge dislocation are calculated. It has been pointed out that the elastic strain agrees well with experimental data found recently for an edge dislocation in graphene.

1. Introduction

A challenging and active research field is the investigation of the material behavior of graphene, especially the study of dislocations in graphene (see, e.g., [2–6]). Graphene is a two-dimensional (2D) material with extraordinary physical properties. In a recent experiment [1], the elastic strain and rotation fields produced by an edge dislocation in graphene have been observed for the first time. It was reported that the lattice rotation is quite appreciable at the dislocation core. Also it was noted that the measured elastic strain contours, do not agree with the corresponding contours calculated in classical elasticity theory. This indicates that a general dislocation continuum theory including the elastic rotation, is needed for a theoretical prediction of realistic strain and rotation contours. Dislocations are critical for understanding plasticity in 2D crystals and predicting mechanical properties. Dislocations are the fundamental carrier of plasticity of materials and little is known about their effect in 2D crystals.

This Letter shows that the so-called dislocation field or dislocation gauge theory (see, e.g., [7–14]) is a promising and excellent candidate to fulfill the requirements mentioned above, and to give contours which agree with experimental data. In [11] a dislocation field theory, which can be considered as the dislocation gauge theory of the three-dimensional translation group $T(3)$ was developed. The idea of a static dislocation field theory, is to use three terms in the general distortion energy density. One term contains the elastic strain and the elastic rotation fields. Another one proportional to the dislocation density tensor having the meaning of dislocation core energy density and a term containing a background stress tensor, which is needed for self-equilibrating of the dislocations. It is important to mention that the force stress tensor is not symmetric anymore. In [11], non-singular solutions for screw and edge dislocations were found. This Letter adopts the framework of [11] in order to formulate a dislocation field theory for two-dimensional materials, which is a gauge theory of the two-dimensional translation group $T(2)$. We suggest using such a dislocation field theory as a 2D dislocation continuum theory for dislocations in graphene. We propose a 2D dislocation field theory, because the strain fields around dislocations differ from those given by classical elasticity with line singularities.

The outline of this Letter is as follows. In Section 2, the fundamental framework of 2D dislocation continuum field theory is presented. In Section 3, the non-singular solutions of the stress and elastic distortion fields are given. In addition, the components of the dislocation density vector and the effective Burgers vector are calculated. The physical features of the obtained solutions are presented in suitable plots. Section 4, concludes our work.

2. Basic framework

In 2D a dislocation is characterized by the Burgers vector which can be in x- and y-directions with components b_x and b_y. There is no z-direction in 2D. For that reason a dislocation in 2D is a point dislocation. The dislocation is located at the dislocation point. In real 2D materials only edge dislocations are possible since

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the Burgers vector is constrained to lie in the xy-plane. The two physical state quantities in the static theory of dislocations are the elastic distortion tensor

$$\beta_{ij} = u_{i,j} - \beta^{\mathrm{P}}_{ij}, \quad i, j = x, y, \tag{1}$$

and the dislocation density vector

$$\alpha_i = \epsilon_{kl}\beta_{il,k}, \tag{2}$$

$$\alpha_i = -\epsilon_{kl}\beta^{\mathrm{P}}_{il,k}, \tag{3}$$

which is the measure how much the elastic distortion tensor β_{ij} and the plastic distortion tensor β^{P}_{ij} are incompatible. $\epsilon_{ij} = -\epsilon_{ji}$, $\epsilon_{xy} = 1$ is the totally antisymmetric second rank tensor. The displacement vector is denoted by u_i and is not a physical state quantity. Since in 2D a dislocation is a point dislocation, there is no Bianchi identity for dislocations unlike 3D where a dislocation is a line defect. Also it holds

$$T_{ijk} = \epsilon_{jk}\alpha_i = \beta_{ik,j} - \beta_{ij,k}, \quad \alpha_i = \frac{1}{2}\epsilon_{jk}T_{ijk}, \tag{4}$$

where T_{ijk} is Cartan's torsion tensor in 2D (see, e.g., [15]).

The deformation energy density consists of three pieces

$$W = W_{\mathrm{el}} + W_{\mathrm{di}} - W_{\mathrm{bg}}. \tag{5}$$

The first piece is the elastic distortion energy density

$$W_{\mathrm{el}} = \frac{1}{2}\sigma_{ij}\beta_{ij}, \tag{6}$$

the second piece is the dislocation energy density

$$W_{\mathrm{di}} = \frac{1}{2}H_i\alpha_i, \tag{7}$$

playing the role of the dislocation core density and finally, the third piece is the background part

$$W_{\mathrm{bg}} = \sigma^0_{ij}\beta_{ij}, \tag{8}$$

containing the contribution of the residual or background stress tensor σ^0_{ij}, fulfilling the condition $\sigma^0_{ij,j} = 0$, needed to equilibrate dislocations.

The specific response fields in the framework of dislocation field theory shall be given for an isotropic, linearly elastic medium. The force stress tensor is defined by

$$\sigma_{ij} = \frac{\partial W_{\mathrm{el}}}{\partial \beta_{ij}} = \lambda\delta_{ij}\beta_{kk} + 2\mu\beta_{(ij)} + 2\gamma\beta_{[ij]}, \tag{9}$$

where the symmetric part, $\beta_{(ij)} = (\beta_{ij} + \beta_{ji})/2$, is the elastic strain tensor and the skew-symmetric part, $\beta_{[ij]} = (\beta_{ij} - \beta_{ji})/2$, determines the elastic rotation. Here μ and λ are the Lamé coefficients. The coefficient γ is an additional material parameter due to the skew-symmetric part of the elastic distortion (the elastic rotation). Thus, γ is the modulus of rotation (see also [11]). The skew-symmetric stress $\sigma_{[ij]}$ is caused by the (local) elastic distortion $\beta_{[ij]}$. In 2D the trace of the elastic distortion tensor is

$$\sigma_{kk} = \sigma_{xx} + \sigma_{yy} = 2(\lambda + \mu)\,\beta_{kk}, \tag{10}$$

due to $\delta_{kk} = 2$. The response to the dislocation density vector is given by

$$H_i = \frac{\partial W_{\mathrm{di}}}{\partial \alpha_i} = c\alpha_i \tag{11}$$

and is the dislocation excitation vector. In 2D, the dislocation density vector is already irreducible with respect to the two-dimensional group of isotropy, $SO(2)$, and it possesses two independent vector components (α_x, α_y) (see, e.g., [15,16]). c is the dislocation modulus. H_i has the physical meaning of a pseudo-moment stress vector (see also, [11]). Since in 2D we have a dislocation density vector, the theory possesses only one dislocation modulus unlike 3D where three dislocation moduli are present. This 2D dislocation continuum field theory contains four material constants: the two Lamé moduli μ and λ, the rotation modulus γ, and the dislocation modulus c. The positive semi-definiteness of W, $W \geqslant 0$, requires the restriction

$$\mu \geqslant 0, \qquad \gamma \geqslant 0, \qquad \mu + \lambda \geqslant 0, \qquad c \geqslant 0. \tag{12}$$

The Euler–Lagrange equations of W with respect to the elastic distortion tensor are given by

$$\frac{\delta W}{\delta \beta_{ij}} = \frac{\partial W}{\partial \beta_{ij}} - \partial_k \frac{\partial W}{\partial \beta_{ij,k}} = 0, \tag{13}$$

which give the fundamental field equations for dislocations, the dislocation equilibrium condition. They read in terms of the response quantities

$$\epsilon_{jk}H_{i,k} + \sigma_{ij} = \sigma^0_{ij} \tag{14}$$

and with Eq. (11)

$$c\epsilon_{jk}\alpha_{i,k} + \sigma_{ij} = \sigma^0_{ij}. \tag{15}$$

Differentiating Eq. (14) with respect to x_j, the force equilibrium condition of the force stress tensor σ_{ij} follows

$$\sigma_{ij,j} = 0. \tag{16}$$

By means of Eq. (2), Eq. (15) takes the following form

$$c(\beta_{ik,jk} - \beta_{ij,kk}) + \sigma_{ij} = \sigma^0_{ij}. \tag{17}$$

Using the inverse constitutive relation for β_{ij}

$$\beta_{ij} = \frac{\gamma + \mu}{4\mu\gamma}\sigma_{ij} + \frac{\gamma - \mu}{4\mu\gamma}\sigma_{ji} - \frac{\nu}{2\mu(1+\nu)}\delta_{ij}\sigma_{kk}, \tag{18}$$

where the 2D Poisson ratio ν is expressed in terms of the Lamé coefficients

$$\nu = \frac{\lambda}{2\mu + \lambda}, \qquad \lambda = \frac{2\mu\nu}{1-\nu} \tag{19}$$

and the trace of the elastic distortion tensor, which gives the elastic dilatation,

$$\beta_{kk} = \beta_{xx} + \beta_{yy} = \frac{1-\nu}{2\mu(1+\nu)}\sigma_{kk}, \tag{20}$$

and Eq. (16), the field equation (17) can be rewritten in terms of the force stress tensor. The result reads

$$c\left[\frac{\gamma - \mu}{4\mu\gamma}\sigma_{ki,jk} - \frac{\nu}{2\mu(1+\nu)}\sigma_{kk,ij} - \frac{\gamma + \mu}{4\mu\gamma}\sigma_{ij,kk} - \frac{\gamma - \mu}{4\mu\gamma}\sigma_{ji,kk} + \frac{\nu}{2\mu(1+\nu)}\delta_{ij}\sigma_{ll,kk}\right] + \sigma_{ij} = \sigma^0_{ij}. \tag{21}$$

Eq. (21) is the fundamental field equation for dislocations in terms of the force stress tensor derived in the framework of dislocation field theory in 2D. Thus, Eq. (21) is the equation of motion for the stress tensor. Eq. (21) will serve exciting solutions for the dislocation fields.

It can be seen in Eq. (21) that the components of the force stress tensor σ_{ij} are coupled in that equation. We can construct two simple, uncoupled, inhomogeneous Helmholtz equations for the trace σ_{kk}, and the skew-symmetric part $\sigma_{[xy]}$. The trace of Eq. (21) gives