FROM GRADIENT ELASTICITY TO ANGSTRÖM-MECHANICS OF DISLOCATIONS

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1. Introduction

In this work, a non-singular theory of three-dimensional dislocations in a particular version of Mindlin's anisotropic gradient elasticity with up to six length scale parameters is presented [1,2,3]. The theory is systematically developed as a generalization of the classical anisotropic theory in the framework of incompatible elasticity. The non-singular version of all key equations of anisotropic dislocation theory are derived as line integrals, including the Burgers displacement equation with isolated solid angle, the Peach-Koehler stress equation, the Mura-Willis equation for the elastic distortion, and the Peach-Koehler force. It is shown that all the elastic fields are non-singular, and that they converge to their classical counterparts a few characteristic lengths away from the dislocation core. In practice, the non-singular fields can be obtained from the classical ones by replacing the classical (singular) anisotropic Green tensor with the non-singular anisotropic Green tensor derived by [1,2]. The elastic solution is valid for arbitrary anisotropic media. In addition to the classical anisotropic elastic constants, the non-singular Green tensor depends on a second order symmetric tensor of length scale parameters modeling a weak non-locality, whose structure depends on the specific class of crystal symmetry. The anisotropic Helmholtz operator defined by such tensor admits a Green function which is used as the spreading function for the Burgers vector density. The anisotropic non-singular theory is shown to be in good agreement with molecular statics without fitting parameters, and unlike its singular counterpart, the sign of stress components does not show reversal as the core is approached. Compared to the isotropic solution, the difference in the energy density per unit length between edge and screw dislocations is more pronounced.

2. Non-singular dislocation key equations

In the considered version of anisotropic strain gradient elasticity theory, the strain energy density is given by

$$\mathcal{W} = \mathcal{W}(e_{ij}, \partial_k e_{ij}) = \frac{1}{2}\, C_{ijkl} e_{ij} e_{kl} + \frac{1}{2}\, D_{ijmkln} \partial_m e_{ij} \partial_n e_{kl} \tag{1}$$

with

$$D_{ijmkln} = C_{ijkl} \Lambda_{mn}\,, \tag{2}$$

where C_{ijkl} is the tensor of elastic moduli and Λ_{mn} is a (symmetric) length scale tensor containing up to six length scales and describes the shape of the dislocation core. Λ_{mn} gives the additional material parameters of gradient elasticity. Here $e_{ij} = (\beta_{ij} + \beta_{ji})/2$ is the elastic strain tensor, $\partial_k e_{ij}$ is the elastic strain gradient tensor (elastic double-strain), $\beta_{ij} = \partial_j u_i - \beta^P_{ij}$ is the elastic distortion tensor, u_i and β^P_{ij} denote the displacement vector and the plastic distortion tensor, respectively. Gradient elasticity is a continuum model of dislocations with core spreading and leads to non-singular elastic fields.

All the famous dislocation key-equations are non-singular in the used version of anisotropic strain gradient elasticity and they read

$$(3)\quad u_i(\boldsymbol{x}) = -\frac{b_i\,\Omega(\boldsymbol{x})}{4\pi} - \oint_{\mathcal{L}} C_{mnpq}\epsilon_{jqr} b_p F_{jnim}(\boldsymbol{R})\,\mathrm{d}L'_r \qquad \text{(anisotropic Burgers equation)}$$

$$(4)\quad \beta_{ij}(\boldsymbol{x}) = \oint_{\mathcal{L}} C_{mnpq}\epsilon_{jqr} G_{im,n}(\boldsymbol{R})\, b_p\,\mathrm{d}L'_r \qquad \text{(Mura-Willis equation)}$$

$$(5)\quad \sigma_{ij}(\boldsymbol{x}) = \oint_{\mathcal{L}} C_{ijkl}C_{mnpq}\epsilon_{lqr} G_{km,n}(\boldsymbol{R})\, b_p\,\mathrm{d}L'_r \qquad \text{(anis. Peach-Koehler stress equation)}$$

$$(6)\quad W_{AB} = \oint_{\mathcal{L}_A}\oint_{\mathcal{L}_B} \epsilon_{jkl}C_{ilmn}\epsilon_{npq}C_{rstp}F_{skmr}(\boldsymbol{R})\, b^A_t b^B_i\, dL^A_q \mathrm{d}L^B_j \qquad \text{(anisotropic Blin's formula)}$$

$$(7)\quad \mathcal{F}_k = \oint_{\mathcal{L}} \epsilon_{kjm}\sigma_{ij} b_i\,\mathrm{d}L_m \qquad \text{(Peach-Koehler force)}$$

where $\Omega(\boldsymbol{x})$ is a non-singular solid angle and b_p is the Burgers vector. They are given in terms of a non-singular Green tensor and a non-singular $\boldsymbol{F}$-tensor.

The results are summarized as follows:

- the theory of incompatible anisotropic strain gradient elasticity delivers a non-singular and parameter-free dislocation continuum theory,
- Green functions and their first derivatives are non-singular,
- the dislocation key-formulas are non-singular, since: singular Green tensor $\rightarrow$ non-singular Green tensor,
- weak anisotropic nonlocality is relevant in the dislocation core.

Moreover, anisotropic strain gradient elasticity contains

- a two-fold anisotropy: anisotropy of the material (bulk anisotropy, C_{ijkl}) and the anisotropy of the core (nonlocal anisotropy, Λ_{mn}),
- characteristic lengths which can be determined from atomistic calculations (DFT) and give the scale where nonlocality is relevant.

References

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