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OptiDis: Toward fast anisotropic DD based on Stroh formalism.

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ABSTRACT

Dislocation Dynamics (DD) simulations in the hypothesis of isotropic elasticity have proved great reliability in predicting the plastic behaviour of crystalline materials. However it is often the case at high temperature (for instance in irradiated BCC iron) that the structural properties of a material will be better described using full anisotropic treatment of the elastic interaction between dislocations.

The computational cost of updating the nodal forces at each time step is $\pi d \varepsilon$ where $d$ is the degree of anisotropy.

On the other hand, past works showed that the anisotropic stress field can be efficiently described using the Stroh axitic formalism.

Willis-Stedls-Lothe

\[ \sigma_{ij} = \frac{1}{V_d} \int_0^V (\mathbf{C}_{\text{Stroh}} \mathbf{x})_{ij} \, dV \]

where Stroh matrices $Q$ and $N$ only depend on $C_{ijkl}$ and $\varepsilon$. They are computed from the eigenvectors of a $6 \times 6$ matrix $N$ depending on $(\nu, \kappa)$ and $(\alpha, \beta)$ where $(\alpha, \beta) = (\varepsilon_{ijkl} A_{ijkl})$. The notations are recalled fig 1 and the stress field reads

\[ \sigma_{ij}(x, t, b) = C_{ijkl} (\mathbf{C}_{\text{Stroh}} \mathbf{x})_{ij} \]

in the collinear case ($\phi = 0$) the expression is slightly more complicated but can be condensed as follows

\[ \sigma_{ij}(x, t, b) = \frac{2}{3} C_{ijkl} (\mathbf{C}_{\text{Stroh}} \mathbf{x})_{ij} \]

The singularity in the limit $r \to 0$ is currently handled using a simple cutoff parameter like the one defined in [6].

Anisotropy ratio

The degree of anisotropy is quantified by the ratio $A = 2C_{ijkl}(C_{11} - C_{12})$. For the BCC $\alpha - FI$, this ratio goes from $A_{di} = 2.3 \mathrm{to} 4.1\pi A_{\text{sym}} = 7.1$.

OptiDis code: Ongoing developments

- Implementation of the farfield (either iso- or anisotropic)
- Efficient analytic integration of the expansion over the target segments
- Derivation of a consistent non-singular theory for the Stroh approach

PERSPECTIVES

- Development of the program OptiDis
- Implementation of the fast multipole method
- Effective computation of forces on dislocation segments in anisotropic elasticity

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In collaboration with CEA Saclay

REFERENCES

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