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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 that 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 computation of the internal elastic forces is by far the most resource consuming step in DD simulations, which is even more true for anisotropic elasticity in the absence of explicit Green's function.

L. Dupuy, J. Soulard and M. Find showed that the approaches summarized in Yin [8] can be accelerated using spherical harmonics expansions of the Stroh matrices. This feature was implemented in the DD code OptiDis in order to power the anisotropic forces computation. Here we recall the formalism and we discuss optimizations, performances as well as motivations for future developments.

ANISOTROPIC MODEL

The stress field created by a dislocation loop \((X, t, \ell)\) at field point \(x\) is given by Mura's formula [6].

\[
\sigma(x) = \varepsilon_{ab} C_{ijab} \varepsilon_{cd} Q_{ncd} \delta(x - X) + \tau_{ijab} \delta'(x - X)
\]

where \(N_{jm,a,b}\) are linear shape functions. The cost of updating the nodal forces at each time step is quadratic and involves the evaluation of 2 line integrals, therefore it is usually the bottleneck of DD simulations. Moreover there does not exist an analytic closed form for the anisotropic elastic Green's function \(G\). Recently Aubry et al. [2] used an integral representation of \(G\) and developed a fast method in order to parametric expansions in order to evaluate the double line integral semi-analytically. On the other hand, past works [6] showed that the anisotropic stress field can be efficiently described using the Stroh axitic formalism combined with the (2) Willis-Steed-Lothe formula for the finite line.

Willis-Steed-Lothe

\[
u_s = \frac{1}{1 + \nu_s} \alpha (C_{ijkl} \delta_{ik} \delta_{jl} - \beta (m Q_{ncd}) \delta_{ik} \delta_{jl} + \alpha (m Q_{ncd}) \delta_{ik} \delta_{jl} + \gamma (m Q_{ncd}) \delta_{ik} \delta_{jl})
\]

where Stroh matrices \(Q\) and \(N\) [5] only depend on \(C_{ijkl}\) and \(T\). They are computed from the eigenvectors of a \(6 \times 6\) matrix \(N\) depending on \(m\) (which is \(\sigma_{ab}\) oriented) and \(n\) (where \(\alpha\) and \(\beta\) are \(C_{ijab}\) related). The notations are recalled fig 1 and the stress field reads

\[
\sigma(x, \theta, \phi) = C_{ijkl} \varepsilon_{ik} \delta_{ij} \delta_{jl}
\]

In the collinear case \((\ell = 0)\) the expression is slightly more complicated but can be condensed as follows:

\[
u_s = \alpha (m Q_{ncd}) \delta_{ik} \delta_{jl} + \gamma (m Q_{ncd}) \delta_{ik} \delta_{jl}
\]

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 \(\Lambda = 2C_{12} / (C_{11} - C_{12})\). For the BCC \(\alpha = F_{\ell}\), this ratio goes from \(4A_{ik} \approx 2.3\) to \(4A_{24} \approx 7\).