OptiDis: Toward fast anisotropic dislocation dynamics based on Stroh formalism
Pierre Blanchard, Arnaud Etcheverry, Olivier Coulaud, Laurent Dupuy, Marc Blétry

To cite this version:
Pierre Blanchard, Arnaud Etcheverry, Olivier Coulaud, Laurent Dupuy, Marc Blétry. OptiDis: Toward fast anisotropic dislocation dynamics based on Stroh formalism. International Workshop on dislocation dynamics simulations, Dec 2014, Saclay, France. <hal-01095322>

HAL Id: hal-01095322
https://hal.archives-ouvertes.fr/hal-01095322
Submitted on 15 Dec 2014

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
OptiDis: Toward fast anisotropic DD based on Stroh formalism.

Pierre Blanchard 1 · Arnaud Etcheverry 1 · Olivier Coulaud 1 · Laurent Dupuy 2 · Marc Blétry 2

1 INRIA Bordeaux-Sud-Ouest, 200 av. de Villeneuve, 33405 Talence Cedex France | 2 INRIA Saclay, 91120 Gif-sur-Yvette, France

ABSTRACT

Dislocation Dynamics (DD) simulations in the hypothesis of isotropic elasticity have proved great reliability to predict 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 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. Fidel 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 \((\mathbf{b}, \ell)\) at field point \(\mathbf{x}\) is given by Mura’s formula [4]

\[
\sigma_{ij}(\mathbf{x}) = c_{ijkl} C_{ijkl}(\mathbf{b}) (\delta_{ij} - \hat{n}_i \hat{n}_j) + n_{ijkl}(\mathbf{x}) \frac{\partial^2 U_{ijkl}(\mathbf{x})}{\partial x_i \partial x_j}.
\]

The nodal force \(f_{ij}^\ell\), acting at the extremities of a finite dislocation line \((\mathbf{b}, \ell)\), is obtained by integration of the Peach-Koehler force \((\mathbf{F}_{PK} = -\frac{\partial U_{ijkl}}{\partial x_i} \mathbf{n}_j} \) over the target line, i.e.

\[
(f_{ij}^\ell)(\mathbf{x}) = \int d\ell \int_{\mathbf{b}_1}^{\mathbf{b}_2} \mathbf{n}_j C_{ijkl}(\mathbf{x}) \, d\mathbf{b}_i
\]

where \(N_{ijkl}\) 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 based on paraxial 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 axiomatic formalism with (2) the Willis-Steed-Louthe formula for the finite line.

Willis-Steed-Louthe

\[
\mathbf{u}_{nm} = \frac{1}{4\pi} \int d\mathbf{ch} C_{ijkl}(\mathbf{b}) [m_{ijkl}(\mathbf{x}) - n_{ijkl}(\mathbf{x})] \mathbf{n}_i \mathbf{n}_j \frac{\partial \phi}{\partial x_m \partial x_n}
\]

where Stroh matrices \(Q, S\) and \(N\) [5] only depend on \(C_{ijkl}\) and \(\mathbf{b}\). They are computed from the eigenvectors of a \(6 \times 6\) matrix \(N\) depending on \(\mathbf{b}\) and \(\phi\) where \((\mathbf{d}_ij)\) are \(\mathbf{C}_{ijkl}(\mathbf{b})\). The notations are recalled fig 1 and the stress field reads

\[
\sigma_{ij}(\mathbf{x}) = C_{ijkl}(\mathbf{b}) \mathbf{n}_j (\mathbf{x}) \mathbf{n}_i (\mathbf{x})
\]

In the collinear case \(d_{ij} = 0\) the expression is slightly more complicated but can be condensed as follows

\[
\mathbf{u}_{nm}(\mathbf{x}) = \frac{1}{(2\pi)^2} \int d\mathbf{b} Z_{nm}\mathbf{b}
\]

The singularity in the limit \(\epsilon \rightarrow 0\) 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 \(\alpha = F_1\), this ratio goes from \(A_{\alpha} = 2.3\) to \(A_{\alpha_{\text{iso}}} = 7.1\).

The degree of anisotropy is quantified by the ratio \(A = 2C_{ijkl}(C_{11} - C_{12})\). For the BCC \(\alpha = F_1\), this ratio goes from \(A_{\alpha} = 2.3\) to \(A_{\alpha_{\text{iso}}} = 7.1\).