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.
Using the Stroh sextic formalism combined with 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 temperatures (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.

It is often the case at high temperature that the degree of anisotropy is quantified by the ratio

\[ \frac{\alpha}{\gamma} = \frac{X_0}{X_1} \]

defined in [6].

Spherical harmonic analysis
Stroh matrices only depend on the orientation of the source, i.e. \( S = X(t, \phi, \theta) \) (see fig 2) hence they can be expanded into spherical harmonics.

\[ X(t, \phi, \theta) \approx \sum_{l=0}^{\infty} \sum_{m=-l}^{l} X_l^m(t, \phi, \theta) Y_l^m(\theta, \phi) \]

where \( Y_l^m \) denotes the well known spherical harmonics and

\[ x_l^m = \int_0^{2\pi} \int_0^\pi X(t, \phi, Y_l^m(\theta, \phi) \sin \theta) \sin \theta \sin \phi \sin \phi \sin \phi \]

are the coefficients of the expansion.

GIVEN STROH MATRICES ARE REAL, THE EXPANSION REDUCES TO

\[ X(t, \phi, \theta) \approx \sum_{l=0}^{\infty} x_l(0, \phi, \theta) Y_l^0(\theta, \phi) \]

On the other hand depending on the symmetries of \( X \) in \( \phi \) or \( \theta \) some coefficients of the expansions are known to be null (potentially a lot). Once these simplifications were done a significant acceleration of the method (see fig 4).

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

REFERENCES

[1] Scal Hex: software library to simulate large scale n-body interactions using the fast multipole method.