Prerequisites

Before complication of the current code (see Makefile) the following free libraries are used:

1. Eigen `http://eigen.tuxfamily.org/index.php?title=Main_Page`
   Just download the library and unpack it to the folder with the main code

2. Alglib `https://www.alglib.net/`

   Download and unpack the library to the folder with the main code. For that, compile a static library by calling the following commands inside the 'src' folder of alglib:

   ```
   g++ -c *.cpp
   ar rcs alglib.a *.o
   ```

   After compilation of the code, paramaters can be changed in the file 'Parameters.txt'. The code employs parallel computation of the gradient and the number of threads should be assigned.

Description

This code presents the computational model of mesoscopic crystal plasticity in 2D. The model is presented in [1] which encompasses the Cauchy-Born rule [3] and crystal symmetry [4]. Utilising a Lagrangian formulation, the current state of the lattice loaded in a hard device is achieved by minimisation of the total potential energy

$$\Pi = \int_{\Omega} \varphi(\mathbf{C}) dV, \tag{1}$$

where Ω is the domain occupied by a crystal in the unreformed configuration. The Cauchy-Green (metric) tensor $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ and deformation gradient $\mathbf{F}$ determine the elastic energy density $\varphi(\mathbf{C})$. The code uses polynomial energy density is defined in [1, 2] which can be adjusted for the crystals with square and hexagonal unit cells.

The computational scheme involves application of the Finite Element Method. To be more precise, N nodes of a generated square grid, representing a crystal sample , coincide with vertices of triangular elements. Therefore, we use linear approximation of displacement fields and minimize the energy $\Pi = \Pi(u_1, v_1, ..., u_N, v_N)$ with respect to nodal horizontal and vertical displacements u_j and v_j, respectively. The minimization is performed by application of the LBFGS algorithm from

References

[1] R. Baggio, E. Arbib, P. Biscari, S. Conti, L. Truskinovsky, G. Zanzotto, and O. Salman. Landau-type theory of planar crystal plasticity. *Physical Review Letters*, 123(20):205501, 2019.

[2] S. Conti and G. Zanzotto. A variational model for reconstructive phase transformations in crystals, and their relation to dislocations and plasticity. *Archive for rational mechanics and analysis*, 173(1):69–88, 2004.

[3] J. L. Ericksen. On the cauchy—born rule. *Mathematics and mechanics of solids*, 13(3-4):199–220, 2008.

[4] G. Zanzotto. On the material symmetry group of elastic crystals and the born rule. *Archive for Rational Mechanics and Analysis*, 121(1):1–36, 1992.