

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

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

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 $\Pi = \Pi(u_1, v_1, \dots, u_N, v_N)$ 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

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