MSE 676 Project progress report

This is a report on our course project. The aim of this project was to study the deformation of polycrystalline grains and thus effectively developing a simulation for uniaxial tensile testing. We will be first studying the theoretical aspects of deformation and then we will apply these in order to develop our own model (mathematical model) for deformation of a polycrystalline material during a particular case of uniaxial tensile test. With relevant theories on plastic deformation and dislocation interactions we can easily approach the problem on a definite path.

Before the onset of plastic deformation, there are certain number of dislocations which are already present in the system. And due to application of elastic stress many more number of dislocations tend to develop from the frank read"s sources. The already formed dislocations act as forest dislocation in the movement of the newly formed mobile dislocation

Plastic deformation according to this model is characterised by the motion of mobile dislocations across the grains , creating a step equivalent to the number of dislocations multiplied by burgers vector. And these dislocations eventually deform the grain and causes plastic deformation.

Thus we can model these moving mobile dislocations to with a control volume formulation, in the dimensions of dislocation we can formulate as conservation equation in the control volume ! The expression will contain a time varying term along with source terms of mobile dislocations.

The interactions between these dislocations is formulated with the following considerations

In polycrystals, the properties of the system are somehow an average value to all the grain considered individually. On a similar note, the deformation of this crystal will also be considered as an number of grains x average value of this deformation; but with a important consideration that the deformation in the grains must be compatible to it's neighbour.

In a polycrystalline aggregate, the deformation of one grain is not independent of the deformation of its neighbor. The compatibility requirements are such that we need to consider the corresponding deformation of adjacent grains during the deformation of the main grain. The microscopic view of this deformation in a single grain have to be also considered. However, due to the mutual interference of neighboring grains and the problem of compatible deformations among adjacent grains, multiple slip occurs rather easily, and, consequently, there is an appreciable work-hardening right at the beginning of straining. In a manner similar to that in single crystals, primary dislocations interact with secondary dislocations, giving rise to dislocation dipoles and loops which result in local dislocation tangles and, eventually, a three-dimensional network of sub boundaries. Dislocations start to glide on preferred slip planes when a shear force starts to act on that plane. The increasing external stress is balanced only by the interaction of these dislocations among themselves and also with various other hindrances which may be present in the form of precipitates, grain boundaries, etc.

Plastic deformation can only occur in a material when there is some permanent deformation occurring within the material, According to theories it can only occur after a stress greater than some critical stress is applied from within. This critical stress is also seen in the schmid's law, In the dimensions of dislocations we can model this critical stress as following.

Critical stress :

For single phase polycrystals, obstacles to dislocation motion are other dislocations, dislocation substructures location walls), precipitates (or secondary particles), and grain boundaries. In other words, there is an interaction between the dislocations in slip i and slip j system. During deformation, dislocation substructures, such as dislocation. In our problem we consider dislocation interactions of FCC material only. Dislocation substructures induce long-range stresses and contribute to an increase in the critical resolved shear stress (CRSS).

Formulation of critical stress

Thus we consider the evolving nature of CRSS , Meaning the CRSS will itself evolve during the subsequent deformation process due to the change in the environment through which the mobile dislocations will be moving. Thus we take this critical stress also to be in the finite element model a variable.

$$\tau_{crss} = \alpha\mu b \times \left(\frac{1}{d_{gr}} \right); \quad dgr = \frac{1}{\sqrt{\varrho}}$$

In addition to the self-interactions of dislocations in the same slip system, there are five categories of interactions between dislocations moving in different slip systems during plastic deformation. For example, there are twelve {111} h110i slip systems for FCC, The dislocation interactions between different slip systems form resultant junctions that hinder the movement of dislocations, leading to latent hardening.

In addition, according to the generalized Taylor relationship propose by Franciosi , The interactions due to dislocation on other slip systems are formulated as :

The most frequent interactions are those that give rise to

1. Lomer–Cottrell (LC),
2. Sessile junctions).
3. Hirth (H),
4. Coplanar (COP),
5. Glissil interaction.

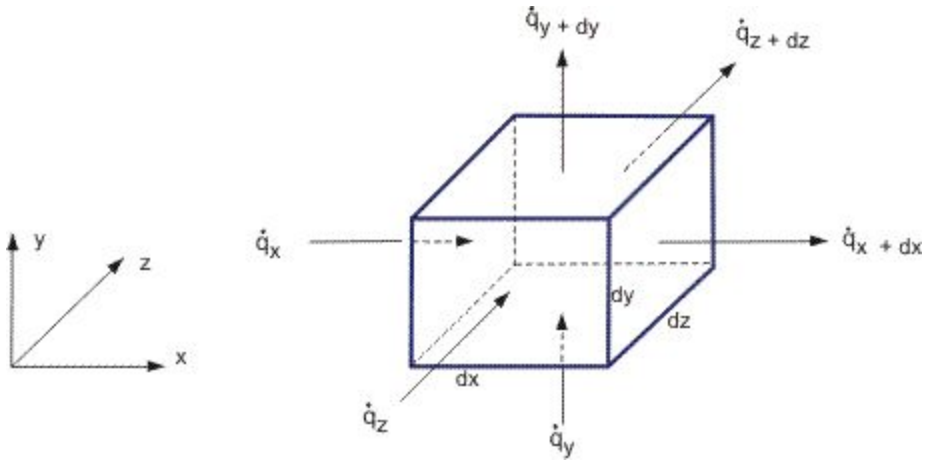
$$\tau_{other(i)} = \mu b \times \sqrt{\sum_{j=1}^{N} \alpha_{ij} \times \varrho_j}$$

Where, i and j are different slip systems ,
alpha i,j are the interactions form of this system.
rho j = density of forest dislocations on this system j.

Solution Scheme

Finite Volume Discretization

In order to make the spatial gradients of dislocation densities and flux densities numerically available and considering a subsequent implementation in a mechanical Finite Element solver we reformulate the above introduced constitutive laws on the basis of a Finite difference discretization.



We assume a control volume in order to perform a mobile dislocation density balance . The faces of the cube introduce the fluxes of the mobile dislocations, Thus account for the influx and outflux of dislocations in the CV. We can also use a generation term, to account for any sources of dislocation.

$$\int_V \frac{\partial \rho}{\partial t}\,\mathrm{d}V + \int_V \operatorname{div} \boldsymbol{f}\,\mathrm{d}V = \sum_r \int_V \dot{\rho}_r\,\mathrm{d}V\ .$$

$$\frac{\mathrm{d}\bar{\rho}}{\mathrm{d}t} = \frac{1}{V}\sum_r \int_V \dot{\rho}_r \,\mathrm{d}V - \underbrace{\frac{1}{V}\oint_{\partial V} \boldsymbol{f}\cdot\boldsymbol{x}\,\mathrm{d}A}_{\dot{\rho}_{\mathrm{flux}}} \ .$$

The first term on the RHS is the source term, assuming that the source term is invariably zero inside the control volume. We are left with this equation.

$$\frac{\mathrm{d}\bar{\rho}}{\mathrm{d}t} = \quad \underbrace{-\frac{1}{V}\oint_{\partial V} \boldsymbol{f}\cdot\boldsymbol{x}\,\mathrm{d}A}_{\dot{\rho}_{\mathrm{flux}}} \ .$$

Now this equation can be formulated by assuming a function for f , f being the mobile dislocation density flux.

.f = (dA.dx x dislocation density x m) / (Acv)xdt

Assuming a uniform distribution of dislocation density flux on this plane the equation reduces to

.f = dislocation density x (v . m)

Where, v = velocity of that dislocation ; m = slip direction

The discretization of the spatial domain into finite control volumes entails an upper bound for the propagation speed of dislocations. Within a time step Δt on average all dislocations that exceed a velocity v1, such that v1*Δt is smaller than the length of the control volume. To ensure that no dislocation can move further than the next neighboring control volume the dislocation velocity should be limited. In the integration scheme though this will be guaranteed by choosing an appropriate time step.

In the context of this work small scale simulation denotes all kinds of simulations, where the element size of the finite element mesh is smaller than the grain size, i.e. each grain is represented by several elements.

Due to its anisotropic nature plastic deformation is never homogeneous on a subgrain scale. First, grains of different orientation are of different stiffness, which leads to strain differences between grains

To account the above model basically, we need to know

- Number of dislocations?
- Interactions between these dislocations ?
- Velocity of this dislocations ?

  All to be answered in the problem formulation.

Final problem formulation

The equation derived from the finite volume model is to be finally solved using numerical techniques, since the Analytical solution will be difficult , The problem takes the shape of a Parabolic equation with space and time derivatives involved in it.

The velocity of the mobile dislocation in the right hand side of the expression is to be written in the form of input variable like applied stress and variables which will affect the motion of this mobile dislocation, which are gibbs free energy for movement of this dislocation , other barriers which will hinder the movement of this dislocation etc.

As mentioned earlier we will consider the critical shear stress formulation and we will directly use it here.

For reducing computational complexity we will consider the following scheme. The slip direction for a particular grain is calculated from the schmid's law and we will only consider that direction for starting our simulation , after this grain is deformed in that direction then only we will consider other direction for deformation.

The line along which the deformation is to be considered is discretized into many small dimensions. As we only want to consider the dislocation density at the boundary of the grain.

The boundary condition and initial conditions are assumed to solve this problem.

Initial condition as zero mobile dislocation at the start of the iteration.
Boundary condition as zero mobile dislocation flux at the boundary.

Code Algorithm

1. We first assumed a random set of grains to make our polycrystalline material.
2. Each grain is numbered such that we can perform our simulation on each of them individually in a given time step.

```
In [16]: import matplotlib.pyplot as plt
         plt.plot((0,2,1,2,0,2,0,5,5,5,5,0,0,0,2,3,3,3,2,2,0,2,0,1,1,2,2,3,2,3,3,5,3,4,3,4,3,3,3,4,4,4,4,4,5,4,5),
                  (5,3,4,5,5,5,5,5,5,0,0,0,0,5,3,5,3,5,3,3,2,0,0,1,1,3,3,1,0,1,1,0,1,2,1,5,1,3,3,5,2,5,3,5,2,2,2,4))
         #plt.plot((1,4),(2,5))
         plt.show()
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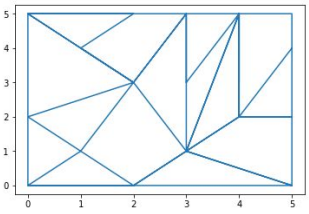


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In [ ]:
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Rest of the algorithm along with the code and the flowchart will be presented in the final report.