Finite Element Method for Simulating Micro-structure of polycrystals during plastic deformation

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1 Introduction

During uniaxial tensile test certain polycrystalline alloys are able to withstand extremely large plastic strains, which is referred to as superplasticity. Several attempts have been made developing the models for superplastic flow accounting for many internal processes such as grain boundary sliding, diffusion, dislocation creep etc,.

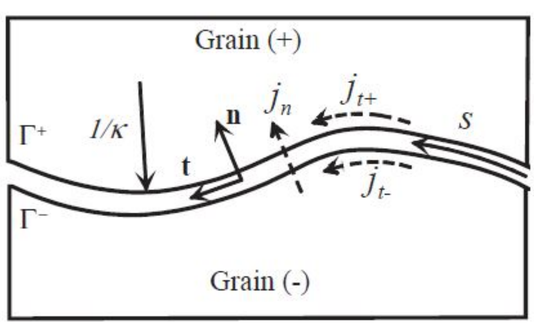
In this project, a similar but simple version of the model considering only the stress driven diffusion of atoms along grain boundaries has been modeled. FEA formulation is done in EN324FEA and the same is implemented in ABAQUS.

2 Model Description

The solid under deformation is idealized as a collection of two dimensional single crystal. In our model we consider one element of the upper grain boundary Γ^+ and the other element from lower grain boundary Γ^-.

The solid is stress free at time t = 0 and then loaded by prescribing the displacements on the upper boundary of the top element $\partial_1 R$ and tractions over the remaining boundaries while keeping lower boundary $\partial_2 R$ fixed. Then the objective is to compute the distribution of the stress across the grain boundary caused by the material flux across the interfaces.

Figure 1: Simple figure describing the model, notation and sign convention



In response to the chemical potential difference, atoms detach from either grain and the resulting flux can be distinguished into three types. The volumetric flux j_n and the two tangential flux j_{t-} and j_{t+} along the grain boundary interface. In our model we ignore the volumetric flux j_n

2.1 Governing Equations

The flux of atoms tangent to each interface is related through

$$j_{t+-} = -\frac{D_{GBt}\delta_{GB}exp(\frac{-Q_{GBt}}{kT})}{2kT}\frac{\partial \mu_{+-}}{\partial s} \tag{1}$$

Total flux tangent to the boundary

$$j_t = j_{t+} + j_{t-} = -\frac{D_{GBt}\delta_{GB}exp(\frac{-Q_{GBt}}{kT})}{2kT}\frac{\partial \mu}{\partial s} \tag{2}$$

Where $\mu = (\mu_+ + \mu -)/2$ and the chemical potential of atoms adjacent to each grain is

$$\mu_{+-} = \Omega\sigma_n \tag{3}$$

Therefore the normal velocity of the grain boundary follows as

$$v_n = \frac{1}{2}(v_{n+} + v_{n-}) = \frac{1}{2}\frac{\partial[j_{t+} - j_{t-}]}{\partial s} \tag{4}$$

$$v_n = \frac{\Omega D_{GBt}\delta_{GB}exp(\frac{-Q_{GBt}}{kT})}{kT}\frac{\partial^2\sigma_n}{\partial s^2} \tag{5}$$

2.2 FE formulation

The finite element approximation for the field is computed using augmented form of virtual work.

$$\begin{aligned}\int_{V_t}\sigma_{ij}(\delta u_i)\delta L_{ij}dV - \int_{\partial V_t} t_i^*\delta v_i ds + \int_{\Gamma_t}(\frac{\Delta u_n}{\Delta t} - \frac{\Omega D_{GBt}\delta_{GB}exp(-Q_{GBt}/kT)}{kT}\frac{\partial^2\sigma_n}{\partial s^2})\delta\sigma_n ds \\ + \int_{\Gamma_t}\sigma_t(\delta v_i^+ - \delta v_i^+)t_i ds + \int_{\Gamma_t}(\frac{\Delta u_t}{\Delta t} - \frac{\Omega\eta_0 exp(\frac{-Q_{GBt}}{kT})}{kT}\sigma_t)\delta\sigma_t ds = 0\end{aligned} \tag{6}$$

On integrating by parts we get the discrete weak form. Here, the continuum part is not shown.

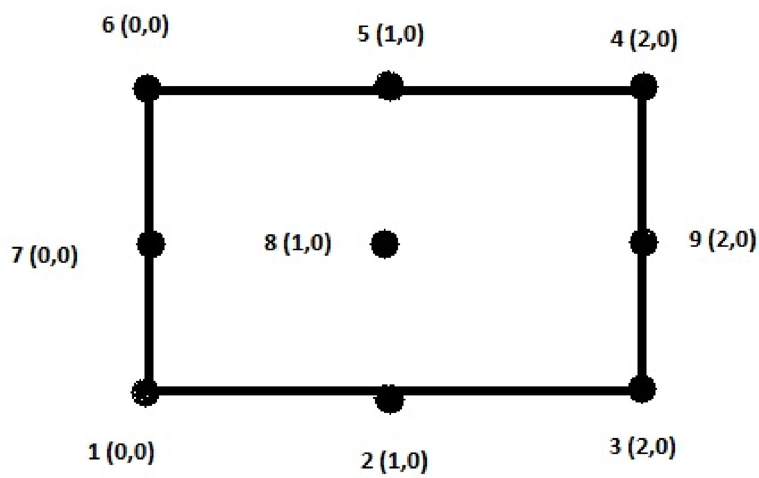
$$\begin{aligned}\int_{\Gamma^e} N^b[N^{a+} - N^{a-}]\sigma_n^b ds + \int_{\Gamma} N^b\frac{\Delta u_n^b}{\Delta t}N^a ds + \int_{\Gamma} C_1\frac{\partial N^a}{\partial s}\frac{\partial N^b}{\partial s}\sigma_n^b ds \\ + \int_{\Gamma} N^b\sigma_t^b(N^{a+} - N^{a-})ds + \int_{\Gamma}[N^b\frac{\Delta u_t^b}{\Delta t} - C_2 N^b\sigma_t^b]N^a ds = 0\end{aligned} \tag{7}$$

Where C_1 and C_2 are constants below and both set to value of 1

$$C_1 = \frac{\Omega D_{GBt}\delta_{GB}exp(\frac{-Q_{GBt}}{kT})}{kT} \qquad C_2 = \frac{\Omega\eta_0 exp(\frac{-Q_{GBt}}{kT})}{kT} \tag{8}$$

The rest of the formulation is similar to the Cahn-Hillard case. Below is the element formulation to solve the problem. The nodes 7, 8, 9 have the tangential and normal stresses as the Degree of Freedom (DOF) while the rest have displacements as DOF.

Figure 2: Element Formulation



Now we define matrices p and B. The B matrix maps the DOFs to the variables in the matrix p

$$p = \begin{bmatrix} \Delta u_n \\ \Delta u_t \\ \sigma_n \\ \frac{\partial \sigma_n}{\partial s} \\ \sigma_t \end{bmatrix} = [B] \begin{bmatrix} u_1^1 \\ u_2^1 \\ u_1^2 \\ u_2^2 \\ u_1^3 \\ u_2^3 \\ \vdots \\ \sigma_t^8 \\ \sigma_n^9 \\ \sigma_t^9 \end{bmatrix} \tag{9}$$

$$B = \begin{bmatrix} N^1 n_1 & N^1 n_1 & N^1 n_1 \ldots N^6 n_2 & 0 & 0 \ldots & & \\ N^1 n_1 & N^1 n_1 & N^1 n_1 \ldots N^6 n_2 & 0 & 0 \ldots & & \\ 0 & 0 & 0 \ldots & N^7 & 0 \ldots & N^9 & 0 \\ 0 & 0 & 0 \ldots & \frac{\partial N^7}{\partial s} & 0 \ldots & \frac{\partial N^9}{\partial s} & 0 \\ 0 & 0 & 0 \ldots & 0 & N^7 \ldots & 0 & N^9 \end{bmatrix} \tag{10}$$

The finite element stiffness matrix and the residual vector can then be expressed as

$$[k^{el}] = \int_V [B]^T [D][B] dV \qquad [r^{el}] = -\int_v [B]^T q dV \tag{11}$$

where

$$q = \begin{bmatrix} \sigma_n \\ \sigma_t \\ \frac{\Delta u_n}{\Delta t} \\ C_1 \frac{\partial \sigma_n}{\partial s} \\ \frac{\Delta u_t}{\Delta t} - C_2 \sigma_t \end{bmatrix} \tag{12}$$

$$[D] = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1/\Delta t & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -C_1 & 0 \\ 0 & 1/\Delta t & 0 & 0 & -C_2 \end{bmatrix} \tag{13}$$

2.3 Analytical Solution

From the earlier discussion C_1 and $C_2 = 1$. Now consider the governing equation (5)

$$v_n = \frac{\partial^2 \sigma_n}{\partial s^2} \tag{14}$$

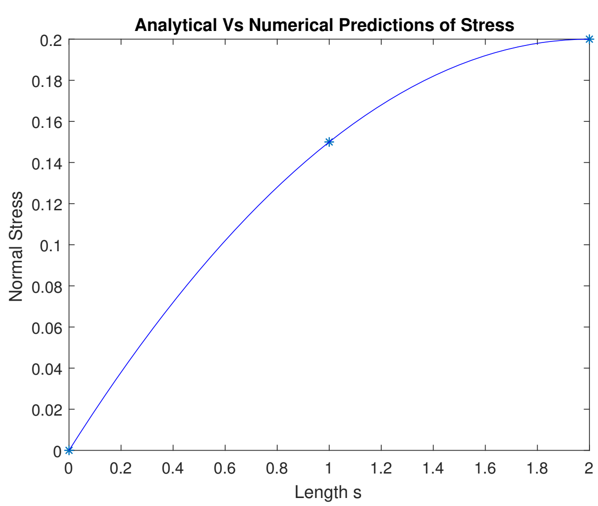
On solving the above equation with the help of below boundary conditions.
$u_1 = u_2 = 0$ for nodes 1,2 and 3. $\sigma_n^7 = 0$, $\frac{\partial \sigma_n^9}{\partial s} = 0$ with the velocity $v_n = 0$ on top nodes 4,5, 6.
The final analytical solution is

$$\sigma_n = \frac{V_n}{2}(s^2 - 4s) \qquad where \quad 0 < s < 2 \tag{15}$$

3 Simulation and Results

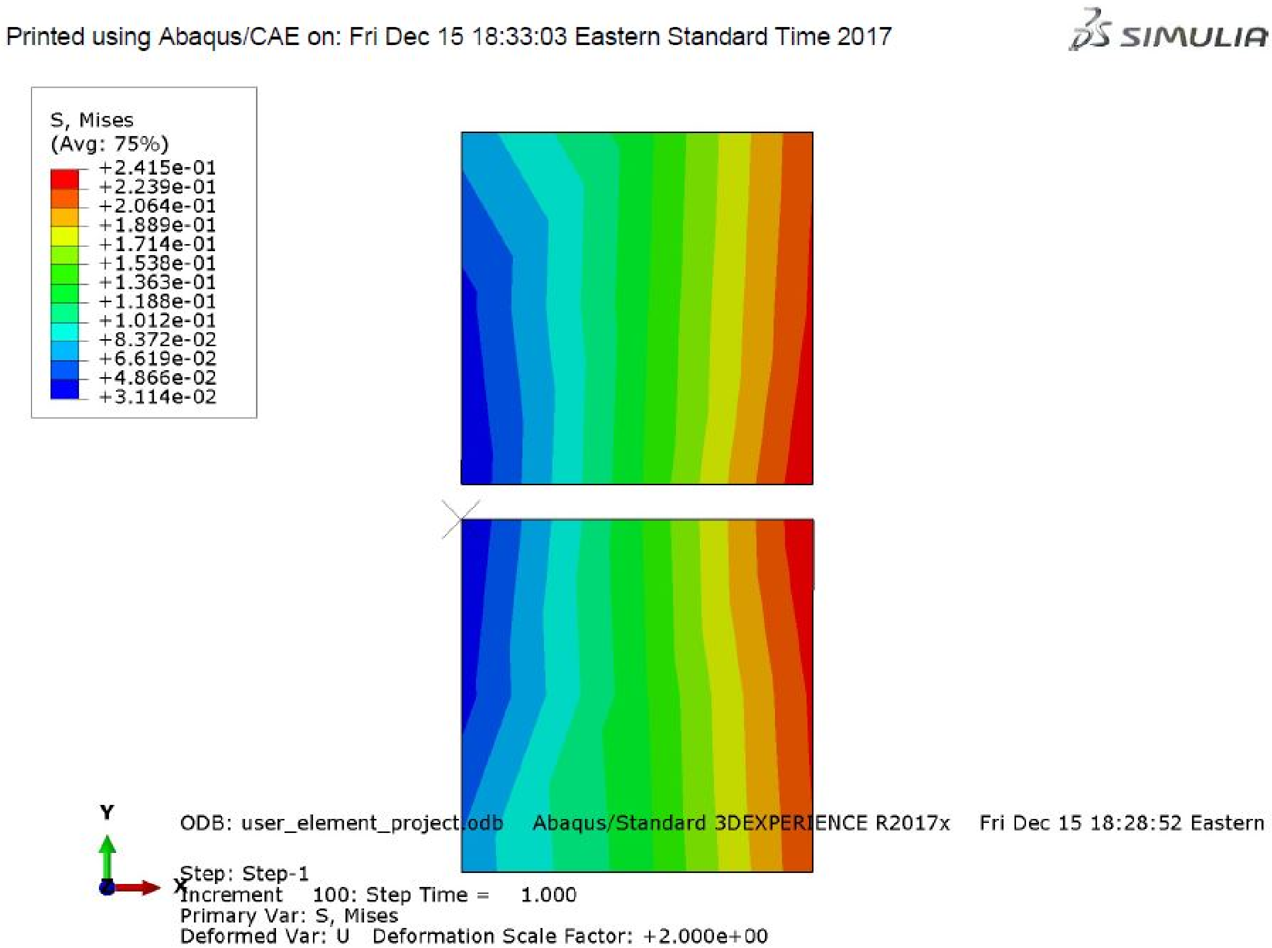
The model is coded as UEL in EN234FEA and a displacements of 0.1 has been applied to the top nodes while the bottom nodes are fixed in both DOFs. $\sigma_n^7 = 0$ and the σ_n^8 and σ_n^9 of the other elements are computed by the simulation. The obtained results should be in conjuncture with the analytical solution. Hence σ_n vs s should be a quadratic curve.

Figure 3: Comparison of the Analytical and Simulated Numerical results



The same model is implemented in Abaqus. Below is the plot of the stress contours. As can be seen the contours are based on the quadratic distribution of the stresses.

Figure 4: ABAQUS simulation results



4 Conclusion & Future Work

In conclusion, the numerical results obtained from EN234 FEA are in conjunction with the analytical results. The normal stress follows the quadratic distribution as obtained in the analytical result. The same is shown in ABAQUS contour plots.

In addition, one can extend the above work to include the volumetric flux, increase the number of elements under consideration, add the boundary migration effects. The same can be implemented in the ABAQUS.

References

[1] Allan F.Bower, Emric Wininger *A two-dimensional finite element method for simulating the constitutive response and microstructure of polycrystals during high temperature plastic deformation*, (Elsevier Ltd, 2003).

[2] ABAQUS Documentation