ENGN 2340 Final Project

Simulating the Plasticity Behavior of Nanocrystalline Cu Using ABAQUS UMAT Subroutine

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1. Introduction

Nanocrystalline metals(NC), which have grain sizes ranging from 1 to 100 nm, have been a hot issue of intensive research for several decades because of their unique physical and mechanical properties [1-3]. However, these materials usually have high strength in the price of relatively lower ductility which has limited the potential of industrial application of NC materials. Therefore, it is significant to study the plasticity property of NC metals, which can help us design and manufacture high quality engineering metal materials.

Finite element method (FEM) has been widely used to simulate and predict the micromechanical behavior of NC metals. In this final project, an ABAQUS user-material (UMAT) subroutine has been written based on the constitutive equations proposed by Zhou et. [4] and the usual viscoplastic constitutive equation learned in class and coded in Homework 10[5-6] to study the mechanical behavior of NC Cu, especially the effect of grain size and strain rate on the global behavior of this material.

2. Material Models

2.1 Mechanism-based gradient plasticity model

A conventional constitutive model for viscoplasticity is provided below to describe the constitutive relation of NC Cu metals.

The strain rate $\dot{\boldsymbol{\varepsilon}}$ can be decomposed into two parts: elastic and plastic part

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}_{\boldsymbol{e}} + \dot{\boldsymbol{\varepsilon}}_{\boldsymbol{p}}$$

The elastic strain rate $\dot{\boldsymbol{\varepsilon}}_{\boldsymbol{e}}$ is obtained from the stress rate in the linear elastic relation as

$$\dot{\boldsymbol{\varepsilon}}_{\boldsymbol{e}} = \boldsymbol{S} : \dot{\boldsymbol{\sigma}}$$

where S is the elastic compliance tensor. The plastic strain rate $\dot{\varepsilon}_p$ is proportional to the deviatoric stress, given as

$$\dot{\boldsymbol{\varepsilon}}_{\boldsymbol{p}} = \frac{3\dot{\varepsilon_p}}{2\sigma_e}\boldsymbol{\sigma}'$$

here $\sigma_e = \sqrt{3\sigma'_{ij}\sigma'_{ij}/2}$ is the von Mises equivalent stress, $\sigma'_{ij} = \sigma_{ij} - \sigma_{kk}\delta_{ij}/3$. $\dot{\varepsilon}_p$is the equivalent plastic strain rate which is determined by

$$\dot{\varepsilon}_{\mathrm{p}} = \dot{\varepsilon}_0 \left[\frac{\sigma_{\mathrm{e}}}{\sigma_{\mathrm{flow}}}\right]^{\mathrm{m}}$$

in which $\dot{\varepsilon}_0$is the material property determined by different materials. m is the equivalent strain rate. m is the strain rate sensitivity exponent; and σ_{flow} is the flow stress that can be expressed in terms of the dislocation densities in the NC fcc metal. The bold font is used to designate tensors.

Many experimental and simulation researches have proved that there exists significant strain gradient near the grain boundary. Dao [7] has defined these area as Grain Boundary Affect Zones (GBDPZ). The thickness of GBDPZ is usually defined as 7-10 lattice constant away from sharp GB, and keeping constant in the plasticity stage. In the present study, we consider d_{GBDPZ} as the thickness of GBDPZ and d_G as the grain size, respectively. According to the descriptions above, the flow stress is related to the volume fraction of GI phase f_{GI} and GBDPZ f_{GBDPZ} in each element, based on the Taylor-type dislocation theory, can be written as follows:

$$\sigma_{\mathrm{flow}} = \mathrm{M}\alpha\mu\mathrm{b}\sqrt{f_{GI}\cdot\rho_{\mathrm{GI}} + f_{GBDPZ}\cdot\rho_{\mathrm{GB}}}$$

Here, ρ_{GI} is the dislocation density in the interior crystal, ρ_{GB} is the one in the Grain Boundary Affect Zones (GBDPZ).

The volume fraction of GI phase f_{GI} and GBDPZ f_{GBDPZ} can be written as

$$f_{\mathrm{GI}} = \left(\frac{\mathrm{d} - \mathrm{d}_{\mathrm{GBDPZ}}}{\mathrm{d}}\right)^3$$

$$f_{GBDPZ} = 1 - f_{GI}$$

2.2 Dislocation density in the grain boundary

Due to the high number of dislocations stored along the GBs, the local strain gradient in the GBDPZ can be introduced to obtain the density of dislocations in the GBDPZ. Thus the density of dislocations in the GBDPZ can be expressed by

$$\rho_{GB} = \frac{k^{GB}\eta^{GB}}{b}$$

where $k^{GB} = 6d_{GBDPZ}/\phi^{GB}d_G$, ϕ^{GB} is a constant, and η^{GB} is the strain gradient relevant to dislocations in the grain boundary, can be defined as

$$\eta^{GB} = \frac{\phi^{GB}n^{GB} \cdot b}{d_G}$$

where n^{GB} is the number of dislocations around the GBs which can be treated as a material constant when the grain size is determined.

2.3 Dislocation density in the grain interior

In the interior of grains, the dislocation interaction determinates the plastic deformation process. Thus the density of these dislocations in the GI obeys the evolution law with plastic strain, described by Kocks and Mecking's model:

$$\frac{\partial \rho_{GI}}{\partial \varepsilon_p} = M\left(\frac{k}{d_G} + k_1\sqrt{\rho_{GI}} - k_2\rho_{GI}\right)$$

where M is the Taylor factor, $k = 1/b$, $k_1 = \psi/b$, $k_2 = k_{20}(\dot{\varepsilon}_p/\dot{\varepsilon}_0)^{-1/n}$. $\psi, k_{20}, \dot{\varepsilon}_0$, and n are constant.

3. ABAQUS UMAT Subroutine

To interpolate the constitutive equation above, a dislocation density based plasticity code has been implemented into Abaqus/CAE in the form of UMAT subroutine. The codes are in the Appendix. The procedure of the stress update part of codes is summarized below.

First, following the usual way, compute the deviatoric strain increment and stress

$$\Delta e_{ij} = \Delta \varepsilon_{ij} - \frac{\Delta \varepsilon_{kk} \delta_{ij}}{3}$$

$$s_{ij}^{n} = \sigma_{ij}^{n} - \frac{\sigma_{kk}^{n} \delta_{ij}}{3}$$

Then compute the elastic predictors

$$s_{ij}^{*} = s_{ij}^{n} + \frac{E}{1+\nu} \Delta e_{ij}$$

$$\sigma_{e}^{*} = \sqrt{\frac{3 s_{ij}^{*} s_{ij}^{*}}{2}}$$

Based on the deduction of Lecture notes 13, using the Euler time integration methods, we can get

$$\sigma_{e} + \frac{3E\Delta \varepsilon_{e}}{2(1+\nu)} = \sigma_{e}^{*}$$

Using the Newton-Raphson methods to solve the plastic strain increment

$$\sigma_{e}^{*} - \sigma_{\text{flow}} \cdot \left(\frac{\Delta \varepsilon_{e}}{\Delta t \dot{\varepsilon_{0}}} \right)^{\frac{1}{m}} - \frac{3E\Delta \varepsilon_{e}}{2(1+\nu)} = 0$$

For the flow stress, the dislocation density in the grain boundary ρ_{GB} can be directly calculated by different material parameters. However, for the dislocation density in the grain interior is more complicated. To calculated the ρ_{GI}, we write another Newton-Raphson in the codes to solve the PDE.

Calculate the stress update

$$\sigma_{ij}^{n+1} = \left(1 - \frac{3E\Delta \varepsilon_{e}}{2(1+\nu)\sigma_{e}^{*}} \right) s_{ij}^{*} + (\sigma_{kk}^{n} + \frac{E\Delta \varepsilon_{kk}}{(1-2\nu)}) \frac{\delta_{ij}}{3}$$

Then use the usual way to calculate the material tangent stiffness.

Finally use the Abaqus/CEA to generate several input files. We use the codes and the input file to conduct our various interesting simulations. The constants used for simulation are listed below.

Table 1. Material parameters used in calculation for Nanocrystalline Cu

Parameter	Symbol	Value
Elastic modulus	E	128GPa
Grain size	d_G	15nm－500nm
Poisson's ratio	υ	0.3
Thickness of GBDPZ	d_{GBDPZ}	3.5×10-9 m
Taylor constant	α	0.2~0.5
Shear modulus	μ	42.1 Gpa
Taylor factor	M	$\sqrt{3}$~3.06
Proportionality parameter	ψ	0.2
Dynamic recovery constant	k_{20}	18.5
Dynamic recovery constant	n	12.5
Geometric factor	ϕ	0.5~1.5
Load strain rate	γ	6×10-1 s-1
Reference strain rate	$\dot{\varepsilon}_0$	0.1 s-1
Burgers vector	b	0.256nm
Number of dislocation	n^{GB}	10
Shear Modulus	μ	23.5GPa

4. Several tests for the codes

4.1 The effect of grain size

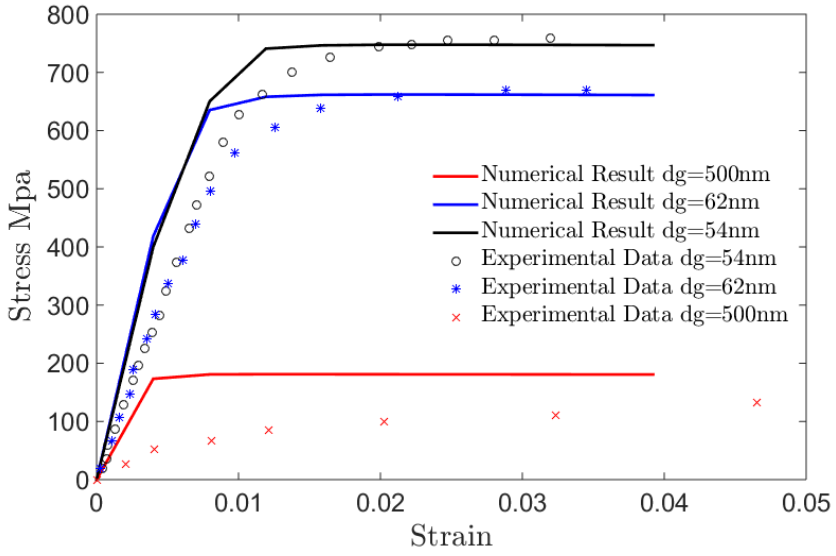

Fig1. Comparison of simulated stress-strain curves with corresponding experimental data [8-9] with grain size of 54nm, 62nm,500nm, respectively.

To test our codes, we compare the numerical result with the experimental data [8-9] with grain size of 54nm, 62nm, and 500nm, respectively. We can find from Fig1. that with the increment of the grain size, the final plastic stress becomes smaller. It is consistent with the famous Hall-Petch relationship. We can also find that the numerical results are consistent with the experimental data especially in plasticity stage for grain size in the nano scale. However, in the course grain size, there is obvious difference between data and numerical result when grain size is 500nm. This is because the governing equation such as the the relationship between dislocation and flow stress in the course grain size is quite different from nano scale. What's more, the simulation shows a little large stress in the elastic stage.

Because we have two different phases, grain boundary(GB) and grain interior(GI), in one grain element, thus studying the role of this two phases take on the plasticity properties

of NC metals can help us gasp the unique mechanism of plasticity in NC metal materials which is different from course grain metals.

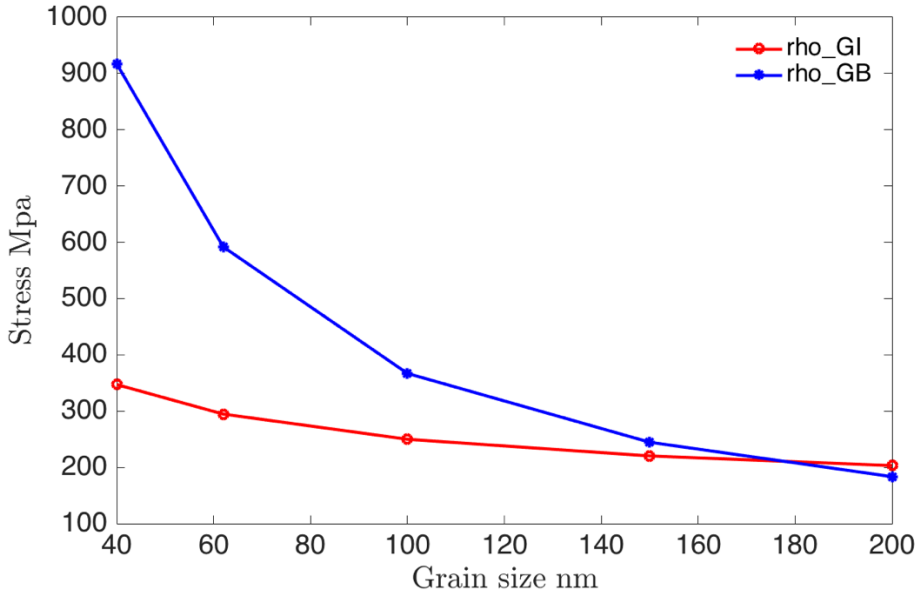

Fig2. The plastic stress with dislocation density exclusively in grain boundary (rho_GB) or grain interior (rho_GI) for different grain size at the true strain of 4%.

To fulfill that purpose, we analyze the effects of dislocation pile-up in GB and GI separately. In Fig.2, the plastic stress caused by dislocation pile-up in GB and GI are simulated separately of different grain size, 40nm, 62nm, 100nm, 150nm, and 200nm at plasticity stage. For plotting simplicity, the stress is chosen when strain is 4%.

We can find that as grain size decreases, both stress caused by the dislocation pile-up in GB and GI are increasing. That is to say, the ρ_{GB} and ρ_{GI} are increasing either. However, ρ_{GB} increases much faster than ρ_{GI} which causes relatively larger stress. When grain size is near 40nm, the stress caused by dislocation pile-up in GB is nearly 3 times larger than in GI. When grain size is larger than the critical size about 180nm, the stress in GI is larger than in GB. However, the stress caused by dislocation pile-up in GB is larger than in GI when grain size is less than 180nm. This is because when grain size reduces to

nano scale, the proportion of GB in one grain element is higher than the proportion of GI compared with course grain metals. This indicates that dislocation pile-up in the grain boundary can be taken as the main carrier of plastic deformation compared with the dislocation pile-up in the grain interior.

4.2 The effect of strain rate

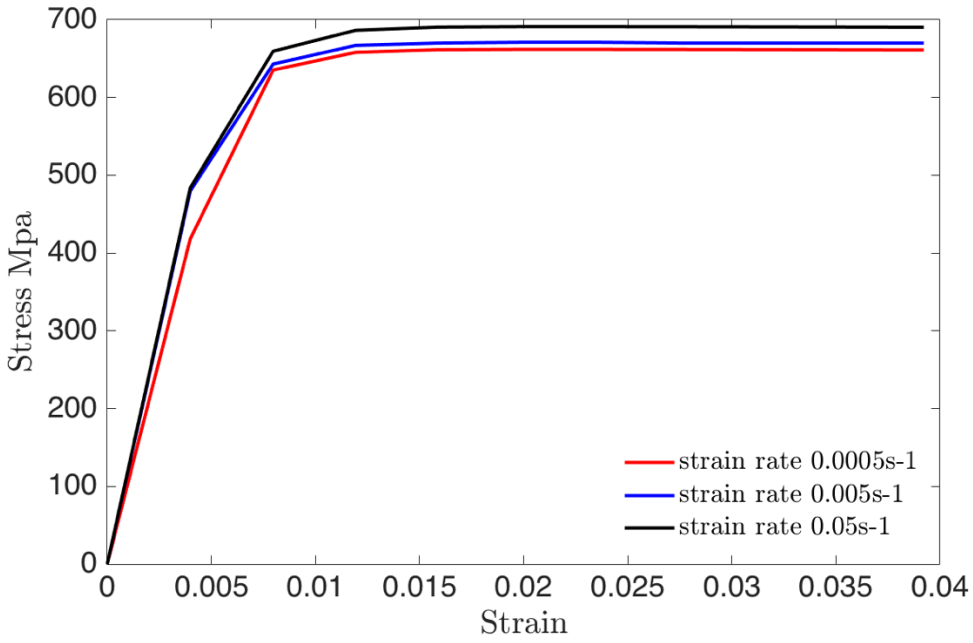

Fig3. Simulated stress-strain curves with strain rate of 0.0005s-1, 0.005s-1, 0.05s-1, respectively.

Much experimental and theoretical analysis has showed that NC metals is rate sensitive. Thus, we simulate the stress-strain curve in different strain rate. We can find from Fig.2 that with the increase of the strain rate, the plastic stress also increases. This simulation proves that the NC metals are rate-dependent.

5. Conclusion

In this final project, an Abaqus/CAE UMAT is written to analyze the plastic behavior of NC Cu materials based on the dislocation density in the grain boundary and grain interior. We find that the simulation results are quite consistent with experimental data especially in plasticity stage. From our simulation, we conclude that in NC metals, when grain size decreases, the plastic stress increases. Moreover, we analyze that it is caused by the relative larger fraction of GB and the dislocation pile-up in GB is the domain reason for NC metals plasticity. Then we prove that the NC metals are rate-dependent.

6. Future work and comments

We can see from the Fig1. there exits difference in elastic stage between experimental data and simulation results. Several approaches have been conducted such as doing the simulation in denser mesh and change the thickness of the grain in the 3D input file. However, there still some difference. Maybe there is some error in the experimental data or the constitutive model proposed by Zhou is not accurate enough. I also doubt the simulation result he did in the paper, which is quite similar to the experiment data in the elastic stage.

Second, NC metals has soft mechanism when grain size is less than 15 nm, which is called revered Hall-Patch relationship. In this project, we haven't considered that mechanism because of limited time. In the later study, we can also simulate the soften mechanism because it is important for small nano scale technology whose grain size is less than 10nm.

Acknowledgement

First, I greatly appreciate Professor Bower for helping me a lot on this course. After doing these 10 assignments and this final project, I begin to be familiar with the mechanism of FEA methods in mechanics. What's more, I gain much coding experience that is very helpful for my future work. Thanks again for Professor Bower debugging for me face to face or via email so many times, and always help me find the deadly bugs.

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