# Finite element modeling of strain rate and grain size dependency in nanocrystalline materials

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**ABSTRACT**

Nanocrystalline materials show a higher strain-rate sensitivity in contrast to the conventional coarse-grained materials and a different grain size dependency. To explain these phenomenon, a finite element model is constructed that considers both grain interior and grain boundary deformation of nanocrystalline materials. The model consist of several crystalline cores with different orientations and grain boundary phase. The nonlinear behavior of the nanocrystalline core is implemented by a grain size dependent crystal plasticity. The boundary phase is assumed to have the mechanical properties of quasi-amorphous material. The constitutive equations for both grains interior and boundary phase are implemented into the finite-element software Abaqus. A calibration procedure was used to tune some parameters of the model with the previously published experimental data on the nanocrystalline copper. Then the model is used to predict the material behavior in various strain rates and grain sizes. The stresses obtained from these simulations match well with the experimental data for nanocrystalline copper at different strains and strain rates. Deviation from the Hall-Petch law and inverse Hall-Petch effect are also well illustrated by the model.

## 1.Introduction

Experimental observations have shown that nano-structured metals exhibit deformation characteristics that are highly sensitive to the rate of loading [1-6]. For example experiments on nanocrystalline (nc) metals reported a more than 10-fold increase in strain-rate sensitivity in contrast to their conventional coarse-grained materials [3, 5]. Rather than this difference strength of ultrafine grained materials tends to deviate from the Hall–Petch law and eventually declines this rule as the grain size reduces to the very fine scale [7-9].

Experimental evidences have shown that when the grain size of polycrystalline metals transits through the micrometer down to the nanometer, there are accompanying transitions in the mechanisms of inelastic deformation [10-11]. It is seemed that both grain interior deformation and grain boundary (GB) deformation mechanisms, including GB diffusion and GB sliding, play important roles in nc materials behavior [7,12]. The variation of strain-rate sensitivity, with grain size and deviation from Hall–Petch law can be explained in terms of deformation mechanisms transitions.

Wei et al [13] explain the enhanced strain rate sensitivity of nc materials in terms of GB mechanisms. There are some models that consider both grain interior and GBs to explain deviation from Hall–Petch law or inverse Hall–Petch effect [14-19]. Kim et al. [20] modeled the

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plastic deformation of nc materials with a constitutive equation based on the evolution of the dislocation density, and included a contribution from diffusion creep (sliding) controlled plastic flow. Anand and Wei [21] introduced cohesive elements along the grain boundaries to model grain-boundary sliding. There are also some micro-macro constitutive models that considers both grain interior and GB deformations [22, 23]. Grain interior deformation in nc materials is believed to occurs due to motion of dislocations (partial and complete) and absorption and emission of dislocations by GBs. In the current work it is assumed that motion of dislocations is the main source of grain interior deformation. However for investigating materials that phase transition is also an important deformation mechanism, the presented constitutive behavior for grain interior should be modified as suggested by Valentini et al [24, 25].

In this paper, a unit cell model is proposed that considers GB deformations as well as grain interior deformation to investigate nc materials behavior. The grains interior deformation is modeled by a grain size dependent crystal plasticity. The increase in flow strength of the grains with reducing grain size is modeled by considering the hardening of individual slip systems a function of grain size. The boundary phase is assumed to have the mechanical properties of quasi-amorphous material and is modeled by an elastic perfectly plastic constitutive law.

The proposed model can well predict nc-Cu strength for various strain rates, strains and grain sizes. Deviation from the Hall-Petch law and inverse Hall-Petch effect for very fine grain sizes are also observed in the results of the model.

## 2.Deformation mechanisms of nc materials

As it is mentioned above studying deformation mechanisms can help to the understanding of the behavior of materials with grain sizes in the range of nanometer. This section introduces some of the proposed physical mechanisms responsible for the specific behaviors in nc materials.

### 2.1. Grain-boundary sliding

In response to shear stress on a grain boundary, two neighboring grains can slide with respect to each other. In conventional polycrystalline metals, grain-boundary sliding only manifests itself at temperatures above half of the material melting temperature. According to the physical experiments, it is proposed that grain-boundary sliding plays a major role in nc metals deformation at ambient temperature.

### 2.2. Grain boundary diffusion

The atoms adjacent to the grain boundary are assumed to be mobile. Atoms may detach from each grain, diffuse along the boundary, and then reattach to one of the two adjacent grains. In this process, the atoms detach from regions of the grain boundary that are subjected to compressive stress and migrate to regions that are under tensile stress [26, 27]. This mechanism not only causes deformation but also help the grain boundary sliding process to produce a consistent deformation.

### 2.3. Grain interior plasticity

In nc material, grain interior plasticity occurs due to both complete and partial dislocations motions as discussed by Zhu et al [28]. Molecular dynamics simulations show that when grain-boundary deformation cannot be accommodated due to geometric restrictions, local stress concentrations develop to cause the emission of a few partial dislocations from grain boundaries, and these high stresses drive the partial dislocations across the grain interiors to be absorbed in the opposite grain boundaries [29].

## 3.Finite element model description

### 3.1. Model geometry and assumptions

In the framework of the unit cell approach, the behavior of materials with complex microstructures is studied by carrying out numerical or analytical studies of the behavior of some cutout of the microstructure. The main assumption, which must be justified, is that the microstructure of whole material can be considered as a periodically repeating microstructure of the cutout, and the cutout is therefore representative for the microstructure of the whole material. Deriving unit cell model for nc material can be done on the basis of a

typical micrograph of the real microstructure. Fig. 1 shows a micrograph of a crystalline material and idealization of it into a structured model. In the final model each hexagonal is representative of a nanocrystal of cu that is randomly oriented due to the global coordinate system. Size of each crystal is equal to the average grain size of the real material. The number of crystals that determines unit cell dimensions should be enough large that model results do not change by repeating the random orientations.

The unit cell model should include grain boundaries rather than crystal cores. The model assumes that grain boundary of a certain thickness exist in it to capture effect of grain boundary mechanisms. The thickness is about 2 nm for all grain sizes [30]. Fig. 2 shows the complete unit cell model with the average grain size of 30 nm.

### 3.2. Constitutive models for various zones of the unit cell

After constructing the unit cell model, material behavior should be assigned to each zone. For all of the crystal cores, a grain size dependent crystal plasticity that is explained in the next section, is used. The only difference between a grain and its neighbor is grain orientation. An elastic-perfectly plastic behavior is used for boundary phase.

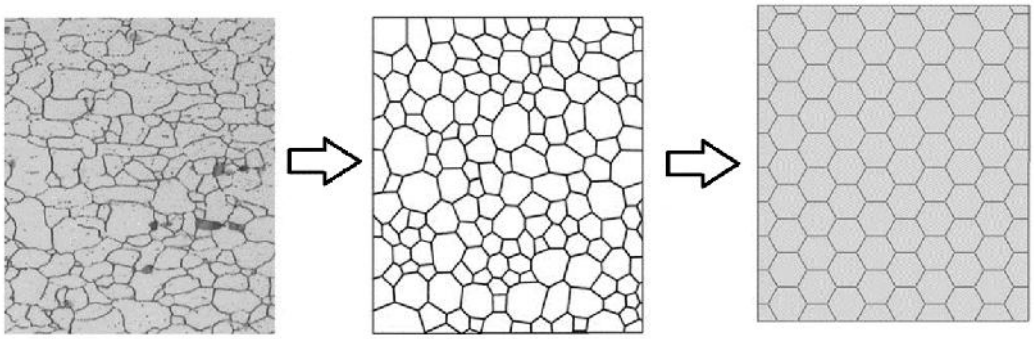

**Fig 1.** Micrograph of a crystalline material and idealization of it into a structured model

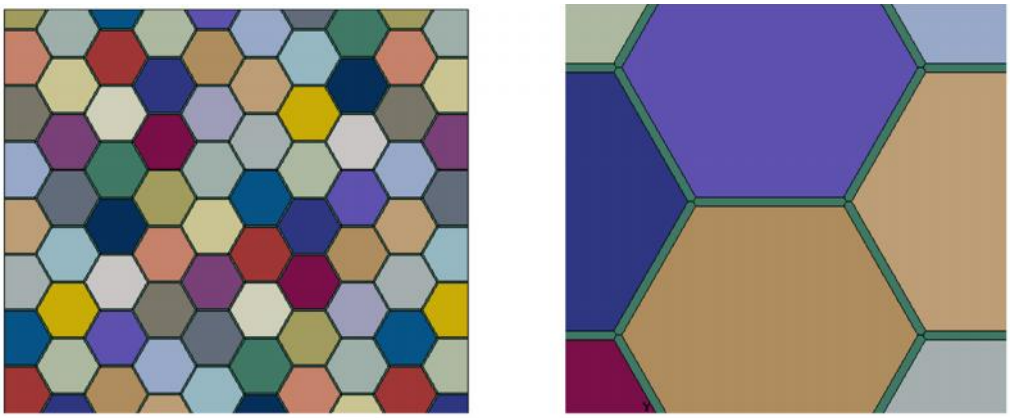

**Fig 2.** Unit cell model considering grain boundaries with the average grain size of 30nm

### 3.3. Material behavior for unit cell model.

#### 3.3.1. Grains interior behavior

Standard crystal plasticity is inadequate to represent the limited amount of inelastic deformation due to emission and eventual absorption of the relatively few (partial or complete) dislocations from GBs in nc materials. However, since the few dislocations in these materials are still expected to move on slip systems, the mathematical structure of continuum crystal plasticity is still useful. Hence, the classical framework of rate-

dependent single crystal plasticity is employed to model grain-interior plasticity. In this paper, Zhu et al. [28] work will be used. In this framework, deformation gradient is decomposed into elastic and plastic parts as:

$$F_{ij} = F^{e}_{ik} F^{p}_{kj} \tag{1}$$

and the velocity gradient and its symmetric and anti-symmetric parts are also decomposed into elastic and plastic parts as:

$$L^{CR}_{ij} = \dot{F}_{ik} F^{-1}_{kj} = \dot{F}^{e}_{ik} F^{e-1}_{kj} + F^{e}_{ik} \dot{F}^{p}_{kl} \dot{F}^{p-1}_{lm} F^{e-1}_{mj} = L^{e}_{ij} + L^{p}_{ij} \tag{2}$$

$$D^{CR}_{ij} = D^{e}_{ij} + D^{p}_{ij} \tag{3}$$

$$W^{CR}_{ij} = W^{e}_{ij} + W^{p}_{ij} \tag{4}$$

The elastic constitutive equation for a crystal is specified by:

$$\hat{T}_{ij} = C_{ijkl} D^{e}_{kl} \tag{5}$$

where $\hat{T}_{ij}$ is the Jaumann rate of Kirchhoff stress tensor considering the lattice rotations, and $C_{ijkl}$ is the elastic moduli tensor. Plastic flow takes place through slip on prescribed crystallographic slip systems, with each system $\alpha$ that is defined by a slip-plane normal $m^{\alpha}_{i}$ and a slip direction $s^{\alpha}_{i}$. The plastic rate of deformation tensor and the spin tensor for the crystal can be respectively written as:

$$D^{p}_{ij} = \sum_{\alpha=1}^{N} \dot{\gamma}^{\alpha} \frac{s^{\alpha}_{i} m^{\alpha}_{j} + s^{\alpha}_{j} m^{\alpha}_{i}}{2} \tag{6}$$

$$W^{p}_{ij} = \sum_{\alpha=1}^{N} \dot{\gamma}^{\alpha} \frac{s^{\alpha}_{i} m^{\alpha}_{j} - s^{\alpha}_{j} m^{\alpha}_{i}}{2} \tag{7}$$

where $\dot{\gamma}^{\alpha}$ is the shearing rate on the slip system $\alpha$ and can be calculated using the rate-dependent law suggested by Asaro and Needleman [31] as:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}^{\alpha}_{0} \left( \frac{|\tau^{\alpha}|}{\tau^{\alpha}_{c}} \right)^{k} \operatorname{sign}(\tau^{\alpha}) \tag{8}$$

here, $\dot{\gamma}^{\alpha}_{0}$ and $k$ denote a reference strain-rate and strain rate sensitivity associated with dislocation motion and $\tau^{\alpha}_{c}$ is the slip resistance to complete dislocations motion and depends on grain size $d$. $\tau^{\alpha}$ is the resolved shear stress on the slip system $\alpha$ and is related to the stress tensor as:

$$\tau^{\alpha} = s^{\alpha}_{i} m^{\alpha}_{j} \sigma_{ij} \tag{9}$$

The grain size dependence of $\tau^{\alpha}_{c}$ is believed to arise mainly from the increasing resistance to nucleation of dislocation loops as the grain size decreases [12]. Therefore, in the current work, it is assumed that initial slip resistance is a constant value for different grain sizes but strain hardening increases as the grain size decreases. The strain hardening is characterized by the evolution of the slip resistance through the incremental relation:

$$\dot{\tau}^{\alpha}_{c} = \sum_{\beta} h_{\alpha\beta} \dot{\gamma}^{\beta} \tag{10}$$

here $h_{\alpha\beta}$ is the slip hardening modulus. The self hardening modulus on each slip system can be calculated using the hardening law suggested by Peirce et al [32]:

$$h_{\alpha\alpha} = h_{o} \operatorname{sech}^{2} \left| \frac{h_{o} \gamma}{\tau_{s} - \tau_{o}} \right| \quad (\text{no sum on } \alpha) \tag{11}$$

here $\tau_{o}$ is the yield stress which equals the initial value of $\tau^{\alpha}_{c}$, $\tau_{s}$ is saturation stress and $h_{o}$ is the initial hardening modulus. The latent hardening can be calculated from:

$$h_{\alpha\beta} = q h_{\alpha\alpha} \tag{12}$$

where $q$ is latent hardening coefficient and in this work $q$=1. In the current work, it is assumed that $h_{o}$ depends on grain size through:

$$h_{o} = \frac{h_{\infty}}{d} \tag{13}$$

here $h_{\infty}$ is the initial hardening modulus of a very large grain. In Eq. 11 $\gamma$ is the cumulative shear strain in all slip systems:

$$\gamma = \sum_{\alpha} \int_{0}^{t} |\dot{\gamma}^{\alpha}| dt \tag{14}$$

In this approach, it is assumed that in grain sizes less than critical grain size $d < d_{c}$ both partial dislocations and full dislocations are active. Therefore, plastic deformation occurs on the 12 {111}(110) slip systems and the 12{111}(112) twin systems of fcc materials.

### 3.3.2. Partial dislocation movement

As the grain size is reduced to a value comparable to the spacing between partial dislocations, plastic flow occurs as a result of partial dislocations emitted from grain boundaries [31]. Since each partial dislocation is trailed by a stacking fault with energy $\gamma_{sf}$, a threshold stress $\tau_{th}$ is required to initiate plastic flow due to partial dislocation movements. Therefore plastic slip rate due to partial dislocation movements could be written as:

$$\begin{cases} \dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha}\left(\dfrac{\tau^{\alpha}-\tau_{th}}{\tau_p}\right)^k & \text{if} \quad \tau^{\alpha} > \tau_{th} \\ \dot{\gamma}^{\alpha} = 0 & \text{if} \quad \tau^{\alpha} < \tau_{th} \end{cases} \tag{15}$$

In this case, the slip resistance will be expressed as [21]:

$$\tau_p = \frac{Gb}{3d} \tag{16}$$

and the threshold stress due to stacking fault energy can be calculated from:

$$\tau_{th} = \frac{\gamma_{sf}}{b_p} \tag{17}$$

here $b_p$ is the Burgers vector of a partial dislocation. The slip systems of Cu when complete dislocations are operative, i.e., $d > d_c$, are the 12 {111}(110) systems. The slip systems when partial dislocations become active, i.e., $d < d_c$, are identical to the 12{111}(112) twin systems of fcc materials. Transition from plastic flow accommodated by complete dislocations to that by partial dislocations can be specified by:

$$\tau_c = \tau_p + \tau_{th} \tag{18}$$

and critical grain size $d_c$ for this transition can be calculated as:

$$d_c = \frac{2Gbb_p}{3\gamma_{sf}} \tag{19}$$

### 3.3.3. Material behavior for grain boundary phase

For the boundary phase, a quasi-amorphous behavior was assumed. The quasi-amorphous behavior of a metal was modeled using an elastic perfectly plastic curve. In this study, we assume the strength of the boundary phase to increase up to an upper limit and then to stay at that level as the grain size or the strain rate increases. Thus no dependence on the grain size or on the strain rate is expected in the behavior of the boundary phase. The stress–strain relation for amorphous materials is considered as ideal plastic behavior, and the assumption of ideal plasticity for the amorphous state is stated to be physically reasonable [20].

### 3.4. Mesh generation, boundary conditions and loading

Fig. 3 depicts the mesh used for the unit cell. The mesh consists of about 35000 bilinear two-dimensional quadrilateral plain strain elements (CPE4R). Plain strain elements were used in order to investigate stress concentration in grains interior and grains boundaries [33]. Study of mesh dependency showed that the mesh size is sufficiently small to reach to reasonable results. In this paper, the UMAT has been written based on plane strain. Stress on each node is achieved after running in the Finite Element Software. The highest stress is captured at the triple junctions of grains. Regarding the [34-37], the stress concentration is created at the junction of two grains because of hardening of nanocrystalline. Since, the principal mechanism of deformation of displacement of dislocation is from one grain to the adjacent grain that leads to slipping crystal planes on each other and deformation of crystal.

The unit cell model will be used to predict the behavior of Cu crystals under tension test in the next section. The boundary conditions required to simulate the uniaxial tension are as follows: as can be observed in figure 4, symmetry conditions are applied on planes x=0 and y=0. There is no traction on planes y=a and the rectangle is subjected to a constant strain rate by displacing the plane at x=a. In this paper, mesh has been demonstrated considering grain boundaries and using implicit solution method. The results for the required number of elements and nodes for mesh are achieved after examining the convergence. If the result in job module is not convergent, the mesh size must be changed until the proper results are attained.

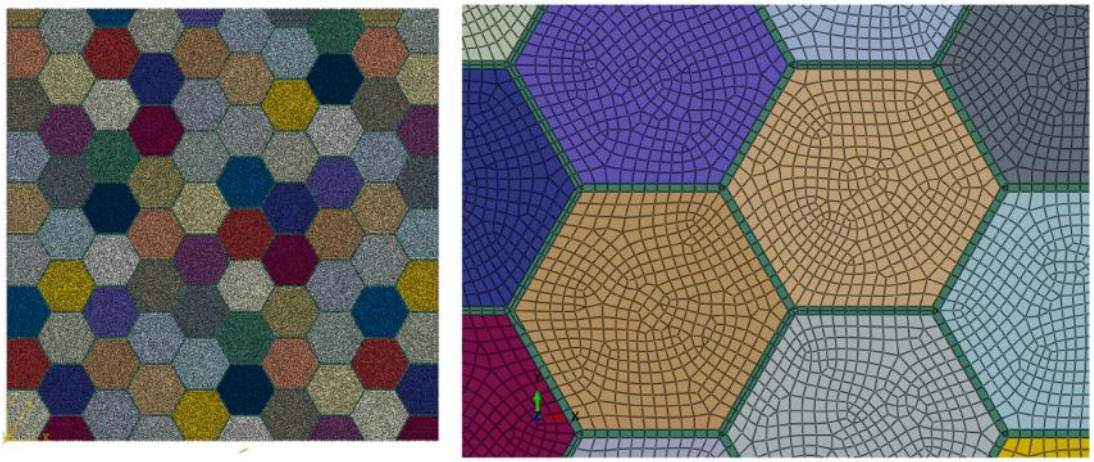

**Fig 3.** mesh generation of the unit cell model

## 4.Results and discussions

In Fig. 5, tensile stress–strain curves of nc-Cu are plotted for seven different strain rates considered in [3]. Similar to the case of coarse grained materials, an increase in the strain rate leads to a harder response of the material but strain rate sensitivity in this case is much higher than coarse grained materials.

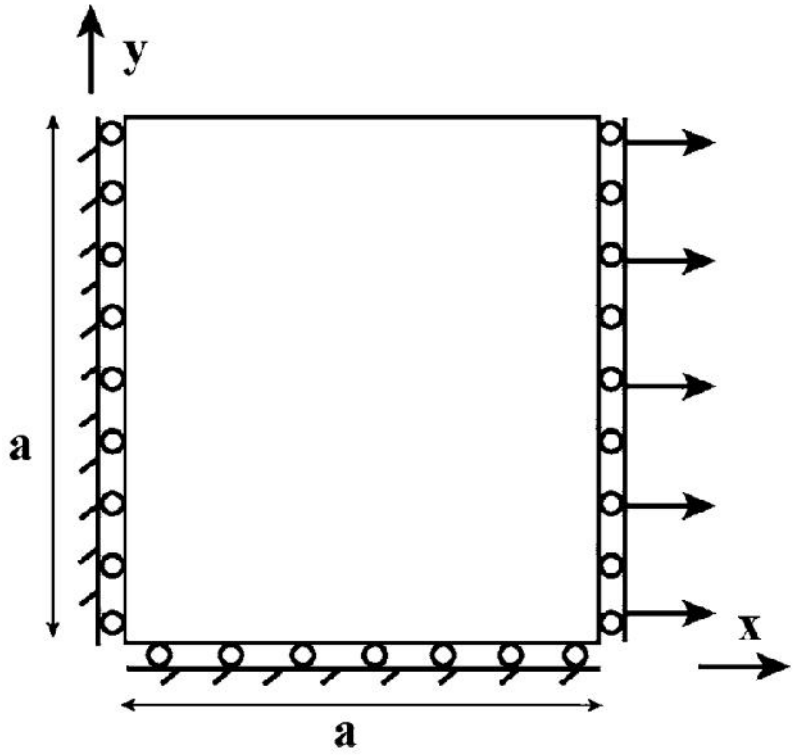


**Fig 4.** the boundary conditions applied to simulate the uniaxial tension

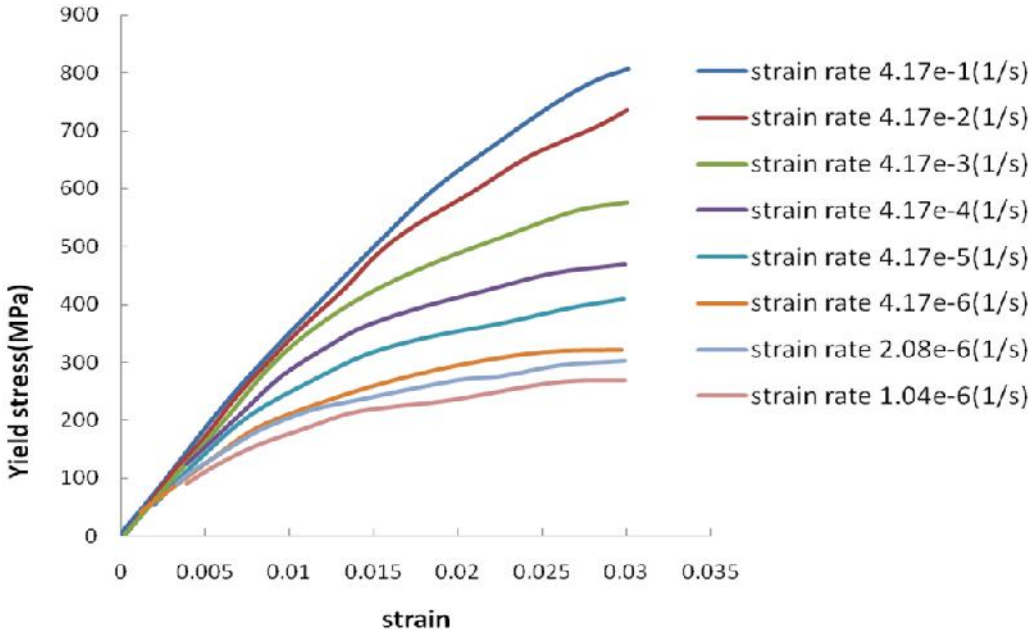


**Fig 5.** Tensile test curves for nc-Cu at various strain rates, due toJiang et al [3]

To model nano-structured polycrystalline Cu, randomly oriented grains are assumed; therefore, the material is initially texture free and isotropic. The values of the parameters listed in table 1 are known for Cu and are used for all simulations in this paper.

Using the simulated model, some stress was obtained for each strain rate which was close to, but not consistent with, experimental results. Therefore, in order to use this achieved model for predicting the real behavior of nanocrystalline Cu in different strain rates, it is required to be calibrated. Thus, based on the properties of each crystal which have been added in the property section and as the material is isotopic; among 160 properties which have been defined for the material, only 6 parameters have been calibrated which are not a lot comparing to the whole number of parameters. Fortunately, the achieved results after calibration were almost consistent with the empirical results and they are practical. The rest of parameters will be obtained from calibration with experimental data due to Jiang et al [3]. In these experiments average grain size is 30nm. The values of these parameters are listed in Table 2.

**Table 1.** values of the known parameters for NC-Cu

| **Parameter** | **Value** |
|---|---|
| Isotropic Elastic parameters [28]: | |
| Isotropic Young modulus E | 135 GPa |
| Isotropic shear modulus G | 40 GPa |
| Stacking fault energy $\gamma_{sf}$ [12]. | 0.045 $Jm^{-2}$ |
| Complete dislocation's Burgers vector *b* | 0.256nm |
| Partial dislocation's Burgers vector $b_p$ | 0.148 nm |
| Critical grain size $d_c$ (Eq. 19) | 16 nm |

**Table 2.** Calibrated parameters used in the simulations

| | |
|---|---|
| Characteristic strain rate $\dot{\gamma}_0$ | $17s^{-1}$ |
| Stress exponent of slip k | 11 |
| Slip system strength $\tau_0$ | 20MPa |
| Saturation stress $\tau_s$ | 770MPa |
| $h_\infty$ | 19000 $Nm^{-1}$ |
| Yield strength of grain boundary | 500MPa |

Comparison between simulation results and experimental data is shown in Fig. 6. The model predicts stresses very close to experiments for various strain rates and strains. Figures 7 and 8 show predicted stress and strain distribution. These figures show while grains interior beer more stresses, grain boundaries deform more than grain interiors. As it was seen in the previous articles [34-37], the triple points are considered as critical points in nano-crystal and in these points we see the maximum tension. In figure. 7. obtained by finite element method software under plain strain conditions, the maximum mises tension is seen around this area. Intensive stress concentration is also observed in triple junctions. To investigate the effect of boundary deformation on the behavior of nc-Cu, a model is constructed without boundaries and results are compared with the model that considers boundaries. Fig. 9 shows stress at the strain rate of 4.17e-1 (1/s) for the mentioned two models. The model without grain boundary shows a higher strength and it can be concluded that by increasing grain boundaries volume fraction at a constant grain size the strength will decreases.

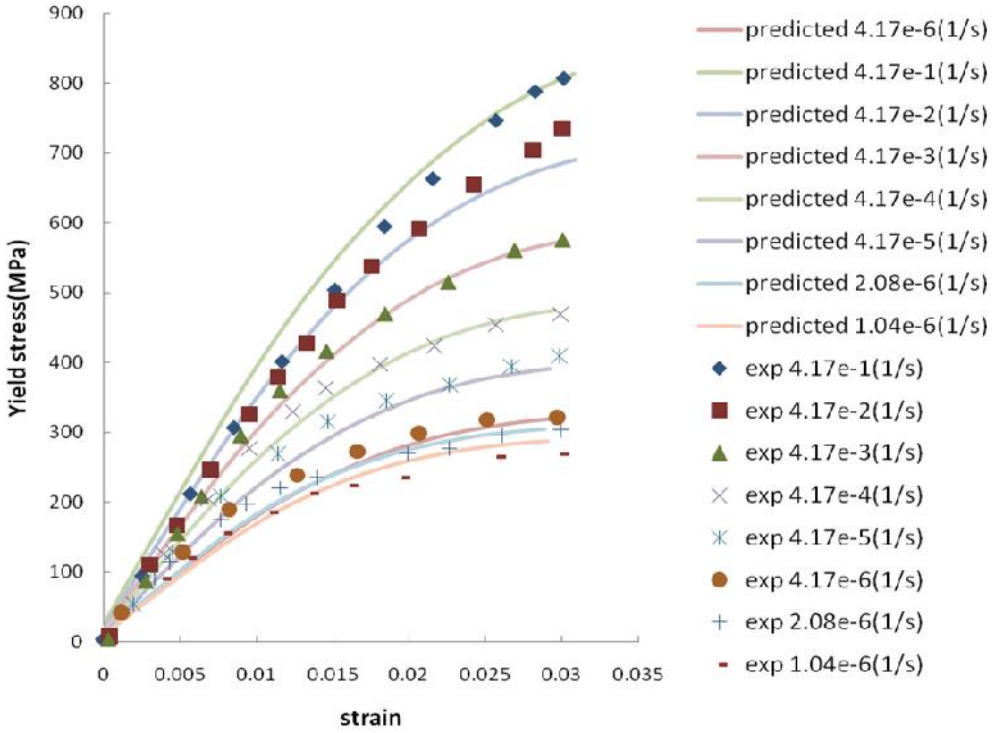


**Fig 6.** Comparison of prediction from the unit cell model with experimental data due to Jiang et al [3]

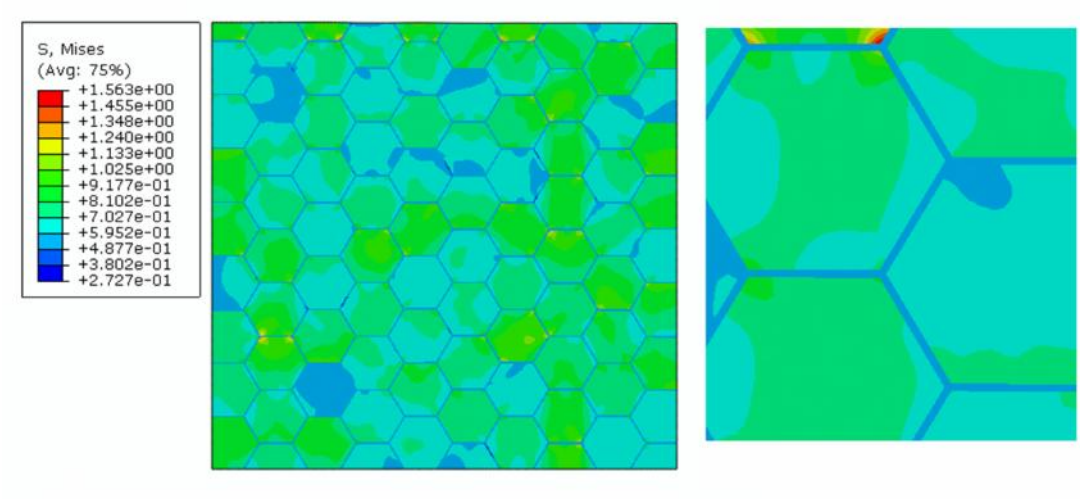


**Fig 7.** Equivalent Misses stress distribution predicted by the unit cell model

To investigate the effect of grain size on nc materials behavior, the model is used to simulate tensile tests with different grain sizes. In these simulations, parameters listed in table 2 are used. Fig. 10 shows the strength of nc-Cu vs. inverse of the grain size square root at the strain rate of 4.17e-3(1/s). The inverse Hall–Petch effect is well captured by current model. By considering figures 9 and 10 simultaneously we can explain what happened in the current model that can capture the inverse Hall–Petch effect and deep our understanding about the nc materials. In a constant grain size increasing the boundary fraction will decrease the strength as is suggested in figure 9. If we want to discuss the role of grain boundary in hardness and yield stress, it is better to compare the model with grain boundary and without grain boundary in terms of quantity. In nano-crystal materials, until they do not reach to critical level, the grain boundaries operate as a bridge for passing of the grains and make nano-crystal harder. This hardness results in the increase of yield stress in the grain, therefore yield stress is higher than the model without boundary.

Without grain boundaries decreasing the grain size will increase the strength. Strength of a real material is a result of these two competing phenomenon. In larger grain sizes (more than strongest grain size) the second phenomena is dominant but in smaller the first causes a reveres behavior.

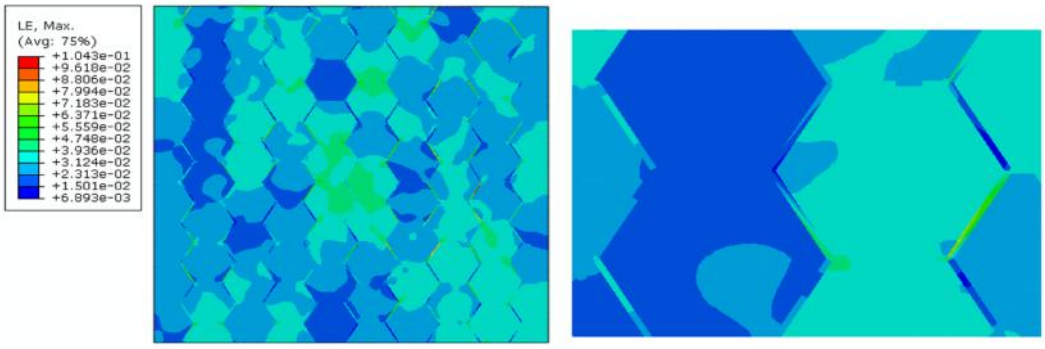


**Fig 8.** Equivalent strain distribution predicted by the unit cell model

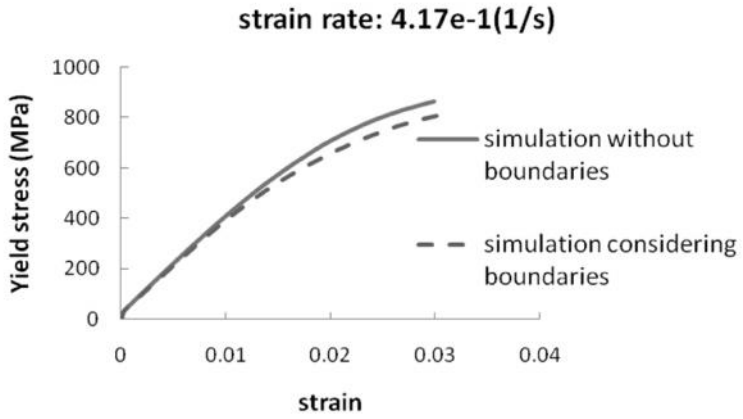


**Fig 9.** Comparison of predicted stress at the strain rate of 4.17e-1 (1/s) for models without and with boundaries

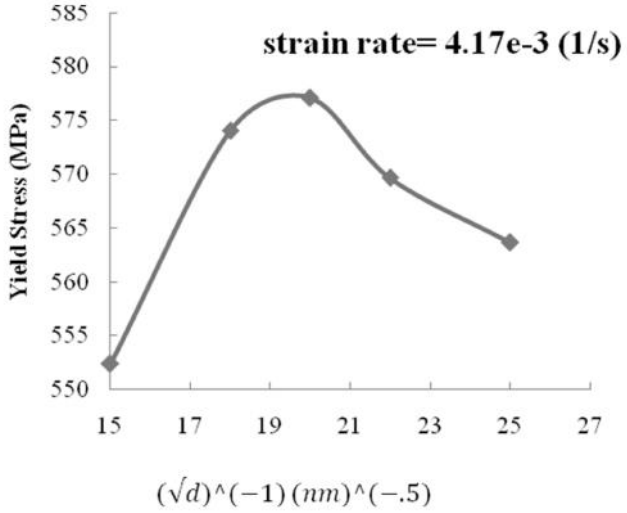


**Fig 10.** Inverse Hall-Petch effect predicted by the model at strain rates of 4.17e-3(1/s)

## 5. Conclusions

In this paper, a unit cell model is constructed to predict nano-crystalline materials behavior for various grain sizes and strain rates. In the model, grain interior plasticity and grain boundaries deformation are considered. Simulation results from the model are in good agreement with tensile test experiments on nc-Cu at different strain rates and strains. The model can well capture two important characteristic of nc materials observed in experiments including enhanced strain rate sensitivity and inverse Hall-Petch relation. Results show that while grain interiors experience more stresses grain boundaries have more deformation. Also a severe stress concentration is observed in triple junctions. The inverse Hall-Petch effect is also understandable base on the grain boundaries role.

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