Finite Element Modelling of the Effects of Average Grain Size and Misorientation Angle on the Deformation

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ABSTRACT

This paper comprises an investigation using finite element analysis to study the behaviour of nanocrystalline grain structures during Equal Channel Angular Press (ECAP) processing of metals. The effects of average grain size and misorientation angle on the deformation are examined in order to see how microstructural features might explain the observed increase in strength of nanocrsytalline metals. While this approach forms a convenient starting as it offers a simple way of including grain size effects and grain misorientation to which we could add additional phenomena through developing the material model used to describe the anisotropy and techniques that would automatically re-mesh the refined grain structure produced under severe plastic deformation. From this, it can be concluded that these additional techniques incorporated into the finite element model produced effects that correspond to observed behaviour in real polycrystals.

Keywords: misorientation, nanocrystalline, anisotropic, grain size, finite element model, Equal Channel Angular Press, von misses stress, microstructural

1. INTRODUCTION

The study of nanocrystalline (NC) metals and alloys has been a topic of research since the 1950ís. These materials have grain sizes typically smaller than 100 nanometres, which are two to three orders of magnitudes smaller than the conventional coarse grained metals (Gleiter, 1989; Kumar *et al.,* 2003; Valiev, 2003).

The mechanical properties of NC materials are found to depend on their structure (Nieman *et al*., 1992) and the meso-structural features such as grain structure, both size and shape, and grain orientation distribution, among other things. The influence of grain size and grain size distribution on the plastic flow stress in polycrystalline materials has been quantitatively described by Hall and Petch in the 1950s based on their work with mild steel (Hall, 1951; Petch, 1953). They observed that the yield strength of polycrystalline mild steel depended on the average grain diameter (Counts *et al.,* 2008). They proposed the following relationship:

$$\sigma_y = \sigma_o + \frac{k}{\sqrt{D}} \tag{1}$$

where σ_y is the yield stress, σ_o is the frictional stress, k is a material constant (Hall-Petch slope) and D is the grain diameter.

The Hall-Petch relationship was established experimentally for the grain size ranges from macro-micro to scale levels. However, recent investigations have shown that it cannot be applied in nano-materials (Wei and Anand, 2004), because the plastic deformation mechanism of coarse Grained metals, intra-grain dislocation slip, is evidentially shut off (Koch, 1992), Instead, smaller levels of strengthening have been observed in UFG solids and softening has been reported in NC solids.

The processing of metals through the application of severe plastic deformation (SPD) has become attractive in recent years as there advantages in comparison to other nanostructured materials (Valiev, 2003). The SPD technique which appears to have the most potential is the Equal Channel Angular Press Technique (ECAP) because it provides the capability of achieving remarkable grain refinement in polycrystalline materials, typically to the submicrometer or even the nanometer level (Valiev *et al.,* 2000). Processing by ECAP leads to significant strengthening of the material at ambient temperatures (Valiev *et al.,* 2002) and the structures obtained have specific features : low density of free dislocations, high angle misorientation of these grains, and high energy and non equilibrium state of grain boundaries (Morita *et al*., 2004).

These structures lead to changes in physical and mechanical properties, a significant increase in the strength with good ductility (Meyers *et al,* .2006). Since the microstructures and the mechanical properties of the deformed materials are directly related to the degree of plastic deformation, the understanding of the phenomena associated with the stress and strain development is very important for a sound ECAP process design to obtain the UFG and NC materials with a good quality by exposing Coarse Grained materials to ECAP (Kim *et al.,* 2002).

Knowledge of the plastic deformation and the load is necessary for understanding the relationships between plastic deformation, grain structures and mechanical properties. In modelling the behaviour of polycrystalline metals and alloy as it is necessary to model both the individual grains (crystals) and their interactions.

The finite element method (FEM) is a process through which a physical structure is translated into a mathematical model and from that mathematical model a numerical procedure is used to approximate the structures behaviour such as deformation, stresses and strains and in some instances the effects of microstructure. The FEM has been widely used in plastic forming process in order to analyse the deformation response of the work-piece with non linear conditions of boundary, loading and materials properties, to compare the effects of various parameters, and to search for best optimum process conditions for a given material and a lot of simulation studies have been done by using different commercial finite element software using 2D or 3D like ANSYS, ABAQUS, DEFORM2, NISA and MSC whereby analysis of the effects of the die angles and frictions between work-piece and channel on deformation behaviour of severe plastic deformation process can be simulated (Zhao *et al.,* 2005).

Much work has already been done on the processing conditions and the resulting behaviours of NC materials and research efforts have been composed of experiment findings, finite element modelling, and various combinations of those efforts. The influence of grain size reduction on the mechanical behaviour of materials has been reviewed in terms of various models.

In this research, an anisotropic elastic-plastic model for the material which was related to the grain structure as each grain was given a different orientation for the anisotropic model was used. These studies were performed on small test meshes at the level of grains after initial macroscopic FE analysis to determine levels of shear strain produced during the ECAP process.

The average misorientation angle was calculated for each grain in terms of the difference between its orientation and the orientations of its neighbours. Both the effect of grain size and high angle misorientation are important phenomena needed to describe the ECAP process.

2. FINITE ELEMENT MODELLING OF ECAP PROCESS

In line with the goals of the research project, the simulations of the extrusion of metals during Equal Channel Angular Press technique was made by assuming isothermal conditions at room temperature and neglecting the heating conditions due to the friction between the work-piece and the die tool to determine the model behaviour of nanocrystalline metals and alloys. The numerical simulations were performed with commercial finite element code ABAQUS/explicit. Three-dimensional finite element analysis was also carried out to explain the deformation process using the deformed geometry. The number of elements used for the simulation is 10877, while the number of nodes is 12489.

The channels angle intersection angles considered for the model is 126°, the outer intersection angle was assumed to be zero. The channels have a diameter of 7.4mm and the die was assumed to be rigid–elastic pieces with element type R3D4 and the material used was a tool steel with young modulus E and the passion ratio V equal to 210,000MPa and 0.3 respectively. The details of the FEM modelling two–dimensional ECAP die tooling with channel angle 126°, are shown in Figure 1 a small fillet radius of 5mm at the inner channels.

Three dimensional work-pieces to have the dimensions of 7.3 mm (width) × 50 mm (height) and a unity thickness with a plane-strain condition are assumed.

Table 1: Material Properties of used

Materials	Young modulus (GPa)	Poisson ratio	Mass density(kg/m^3)
ECAP die	210	0.3	7800
Billet	108	0.31	8940

A displacement boundary condition was imposed on the top line of the work-piece. The compressive displacements imposed on the work-piece top region in the vertical direction were fixed in increment of 0.50 mm up to a total displacement of 40mm in the direction of movement of the punch with a force of 70 kN.

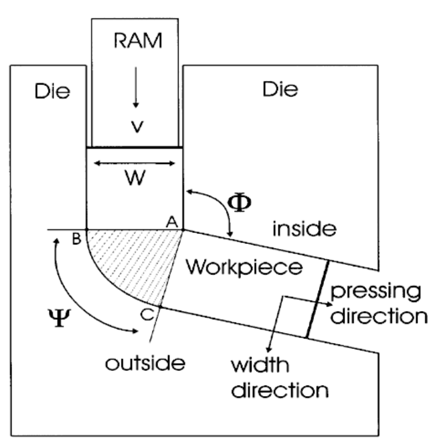

Figure 1: Schematic illustration of the ECAP process showing the die channel angle geometry. Pressing direction, width direction and thickness direction

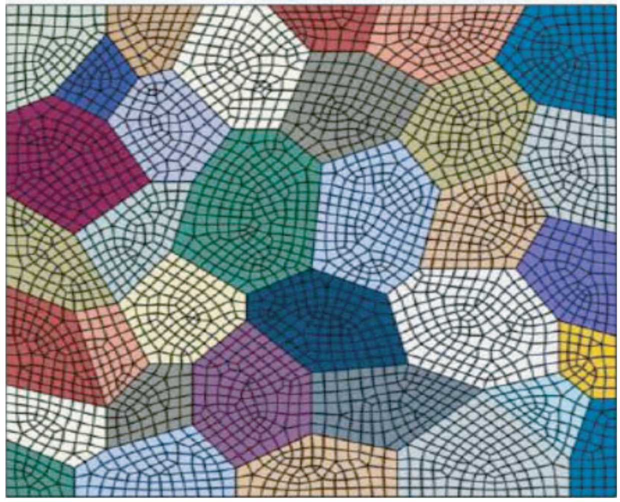

Figure 2: Finite element mesh for Grain size set

3. FINITE ELEMENT MODELLING OF GRAIN STRUCTURE

The grain structures are modelled explicitly using planar tessellation for evaluation of a representative volume element size (RVE) with different grain sizes and randomized grain orientations. The constitutive model of crystal grains utilizes anisotropic elasticity and plasticity and the finite element method is applied to solve the boundary value problem defined at the macroscopic scale. Fortran programs were used to assign random angles for grain anisotropy and to compute the average misorientation angle for grains and neighbouring grains. The grain size is also computed so that both the grain size and misorientation angles can be related to the stress distribution. The grains are randomly sized and shaped. The aggregates contain 34 grains tessellation analysed. The deformations considered in this model are simple shear. The displacement u is applied in the $+X_1$ direction to the top of the unit cell and the whole length of the bottom edge is fixed in the X_1. The unit cell is shear by $\varepsilon = 0.20$ and $\overline{u} = 17$ microns for grain size set 1 aggregates.

The different colours indicate grains in the microstructure with a specific crystallographic orientation for each grain. The analysis is limited to two Dimensional structures due to the high computations efforts. Crystallographic orientation is assigned randomly to each grain in the model to investigate the plastic deformation. The grain orientation varies from grains to grain for a given crystallographic orientation set. This is done to assess the size effect only. The tessellations and randomly distributed grain orientations are set at the start of the analysis and mapped to the finite element discretization.

Table 2: shows the set assigned with orientation angles

Orientation set	**Orientation angle**
Set A	22.5
Set B	45
Set C	90

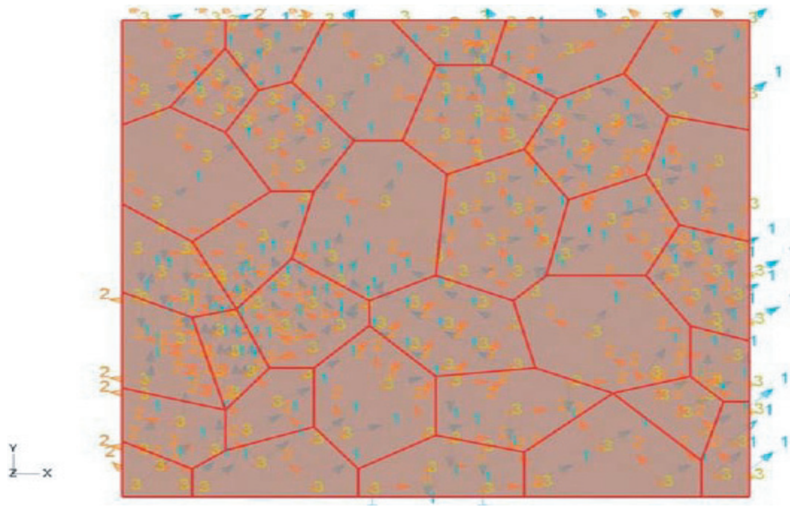

Figure 3: tessellation with highlighted orientation of grains for Grain size

The micromechanical models homogenous traction and displacement boundary conditions used are according to:

$$\sigma(\vec{x})|_{\partial V} = \sigma_0 \cdot \vec{n}(\vec{x}) \tag{2}$$

$$\vec{u}(\vec{x})|_{\partial V} = \varepsilon_0 \cdot \vec{x} \tag{3}$$

Table 3: Grain size set 1 with orientation angle

Grain	Orientation angle
1	0.0617999807
2	40.1232948
3	33.2319107
4	24.4384594
5	40.4913483
6	26.9859924
7	20.0369282
8	36.2985611
9	14.7015295
10	25.153965
11	7.63161087
12	38.7128792
13	17.3754082
14	0.832239747
15	44.1567726
16	24.4851532
17	40.9431763
18	41.7039986

Table 3: Grain size set 1 with orientation angle (Continued)

Grain	Orientation angle
19	9.14365005
20	39.773098
21	15.1602221
22	41.3167191
23	25.9793396
24	9.84267712
25	20.4557934
26	32.1909218
27	8.1878109
28	3.32895899
29	40.803093
30	10.3164768
31	11.6019163
32	13.8637953
33	39.4174004
34	6.16489172

Table 4: Connectivity inputted for Grain size

Grain							
1	2	7	12	0	0	0	0
2	1	7	3	8	0	0	0
3	2	4	9	13	8	0	0
4	3	9	5	0	0	0	0
5	4	9	10	6	0	0	0
6	5	10	11	0	0	0	0
7	1	12	8	2	0	0	0
8	2	7	12	30	13	3	0
9	4	3	13	14	10	5	0
10	5	9	14	15	11	6	0
11	6	10	15	16	0	0	0
12	1	7	8	30	27	0	0
13	9	3	8	30	19	20	14
14	9	13	20	21	0	0	0
15	10	11	20	21	15	10	0
16	11	15	21	22	0	0	0
17	27	18	23	0	0	0	0
18	27	17	23	0	0	0	0
19	13	30	18	24	31	20	0
20	14	13	19	31	29	21	0
21	16	15	14	20	29	26	22
22	16	21	26	34	0	0	0
23	17	32	33	24	0	0	0
24	31	19	18	23	33	0	0
25	26	34	29	28	0	0	0
26	22	21	25	34	0	0	0

Table 4: Connectivity inputted for Grain size (Continued)

Grain							
27	30	18	17	0	0	0	0
28	29	25	31	33	0	0	0
29	21	20	31	28	25	0	0
30	8	12	27	19	13	0	0
31	20	19	24	33	28	29	0
32	23	33	0	0	0	0	0
33	31	24	28	0	0	0	0
34	26	25	22	0	0	0	0

Table 5: Number of connected grains with misorientation angle for Grain size

Grain							
1	2	7	12	0	0	0	0
2	1	7	3	8	0	0	0
3	2	4	9	13	8	0	0
4	3	9	5	0	0	0	0
5	4	9	10	6	0	0	0
6	5	10	11	0	0	0	0
7	1	12	8	2	0	0	0
8	2	7	12	30	13	3	0
9	4	3	13	14	10	5	0
10	5	9	14	15	11	6	0
11	6	10	15	16	0	0	0
12	1	7	8	30	27	0	0
13	9	3	8	30	19	20	14
14	9	13	20	21	0	0	0
15	10	11	20	21	15	10	0
16	11	15	21	22	0	0	0
17	27	18	23	0	0	0	0
18	27	17	23	0	0	0	0
19	13	30	18	24	31	20	0
20	14	13	19	31	29	21	0
21	16	15	14	20	29	26	22
22	16	21	26	34	0	0	0
23	17	32	33	24	0	0	0
24	31	19	18	23	33	0	0
25	26	34	29	28	0	0	0
26	22	21	25	34	0	0	0
27	30	18	17	0	0	0	0
28	29	25	31	33	0	0	0
29	21	20	31	28	25	0	0
30	8	12	27	19	13	0	0
31	20	19	24	33	28	29	0
32	23	33	0	0	0	0	0
33	31	24	28	0	0	0	0
34	26	25	22	0	0	0	0

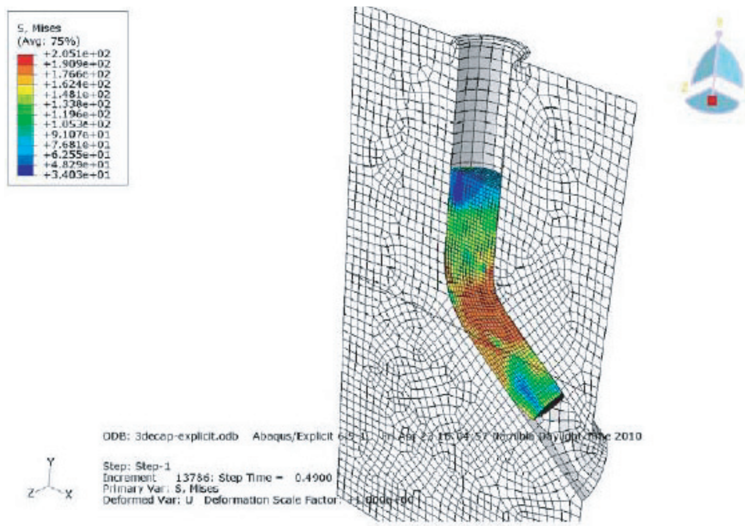

Figure 4: Von Mises distribution obtained with 3D geometry

3.1. FINITE ELEMENT SIMULATION RESULTS

In order to investigate the stress distribution value, finite element simulations were carried out for the ECAP process of copper alloy. Fig 4 shows the Von Mises stress distribution obtained with 3D geometry at the exit. From the deformed geometry, it can be seen from the stress distribution that the stress at the inner part is different from that in the outer side due to the difference in the deformation history. The inner part of the entry side receives compressive stress due to the compression of the plunger, and the maximum compressive stress appears in the inside corner. The center part and the inner part of the billet are heavily sheared, but the outer part appears to be much less sheared this can attributed to the frictional effect between the billet and the die.

To illustrate the effects of misorientation angle on grain structures during deformation Fig. 5, 6, and 7 shows the simulations result for grain structures with orientation angle of 22.5°, 45° and 90° respectively during ECAP process. From Table 6 which shows the Average misorientation angle, maximum and minimum stress for the grain structure it was observed that the maximum and the minimum stress distribution for all the sets are difference, it is due to the orientation and misorientation angle assigned to the grains since the same condition was used for simulating.

3.2. CONCLUSION AND DISCUSSIONS

We have thus successfully demonstrated a relatively efficient finite element technique which makes the stress field dependent on the grain size and the angle of misorientation between grains. This approach is for example more efficient and much simpler than the techniques developed by other researchers to apply crystal plasticity models to the finite element modelling of polycrystals. It is also easier to relate the model to real materials as it is possible to measure both grain size and the average misorientation angles physically and incorporate them into the model without having to use sophisticated methods to find model parameters.

The results have been analysed in terms of the influence of grain size and misorientation angle on the stress distribution and average stress. The simulated results show that the grain size and the grain misorientation angle have significant effects on the stress distribution and average stress within the polycrystalline area.

Table 6: Misorientation angle, each grain area, maximum and minimum stress for set 3 at orientation set C

Grain	Misorientation angle	Grain area (Microns)	Maximum stress (MPa)	Minimum stress (MPa)
1	65.791	64.917	1.223E02	2.346E01
2	35.431	121.9725	1.223E02	9.434E01
3	21.255	108.52	1.083E02	6.635E01
4	23.055	31.936	1.223E02	1.223E02
5	35.342	75.334	1.233E02	1.223E02
6	23.127	89.759	1.233E02	6.635E01
7	37.499	29.374	1.36E02	1.036E01
8	23.490	73.43	1.083E02	9.434E01
9	277.018	93.536	1.233E02	8.035E01
10	29.499	95.3838	1.233E02	6.635E01
11	45.128	81.9745	1.233E02	8.035E01
12	47.461	109.633	2.436E01	1.036E01
13	26.196	139.88	1.223E02	1.083E02
14	50.442	120.2527	9.434E01	8.035E01
15	44.454	78.2193	6.635E01	3.835E01
16	31.341	69.584	1.223E02	1.083E02
17	32.320	64.997	1.223E02	1.223E02
18	49.349	34.9226	1.36E02	1.36E02
19	25.250	78.325	1.083E02	8.035E01
20	48.594	101.6152	1.643E02	1.3636E02
21	41.740	137.1667	1.223E02	6.635E01
22	43..633	31.432	1.083E02	1.363E02
23	28.327	49.631	1.783E02	1.363E02
24	32.012	44.628	1.783E2	1.503E02
25	31.750	106.884	1.783E02	1.363E02
26	31.959	38.5531	1.503E02	1.363E02
27	45.600	46.04275	9.434E01	1.223E02
28	49.481	68.507	1.22E02	6.635E01
29	45.478	84.894	1.643E02	1.363E01
30	25.896	63.5838	9.434E01	8.035E01
31	32.559	154.134	1.643E02	1.503E02
32	37.669	24.54	1.783E02	1.363E02
33	62.319	71.034	1.643E02	1.363E02
34	50.312	32.7307	1.363E02	3.835E01
The mean grain size	37.669	76.9802	127.368	92.7426
Standard deviation	11.056	34.63156	33.000	42.841

The plasticity was model without hardening in order to isolate the effect of grain size with misorientation angle from other effects such as kinematic hardening in anisotropic grains, if we add kinematic hardening to randomly distributed misorientation of the anisotropic grains we might get similar effects to the dislocation pile up which is said to be part of the inverse Hall-Petch mechanism as described in the thesis.

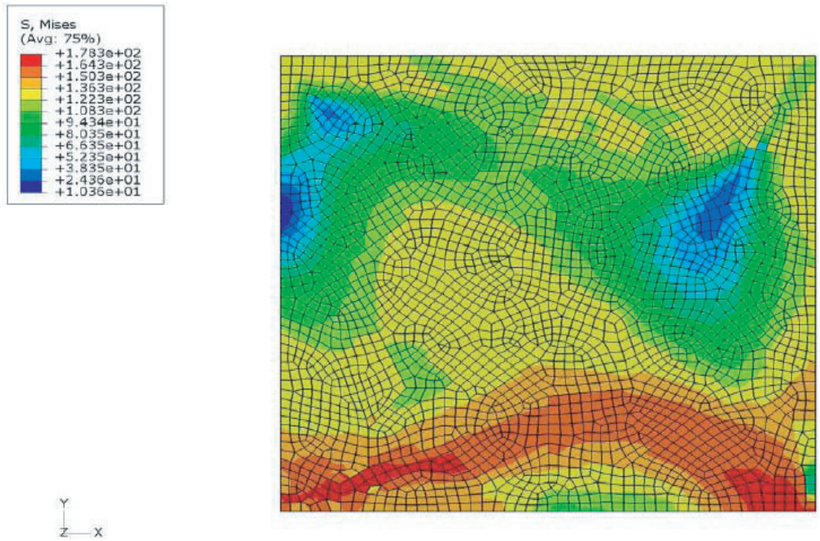

Figure 5: Equivalent stress for grain size set 1 with assign random grain orientation angle of set A after simple shear.

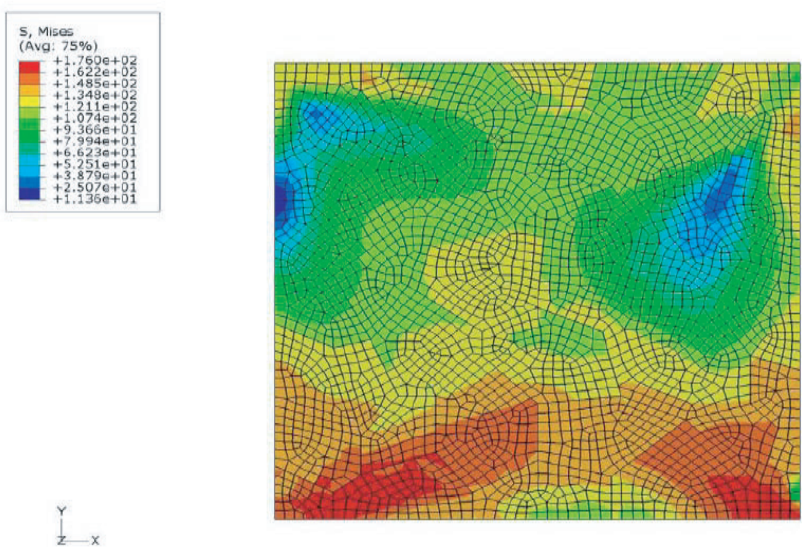

Figure 6: Equivalent stress for grain size set 1 with assign random grain orientation angle of set B after simple shear.

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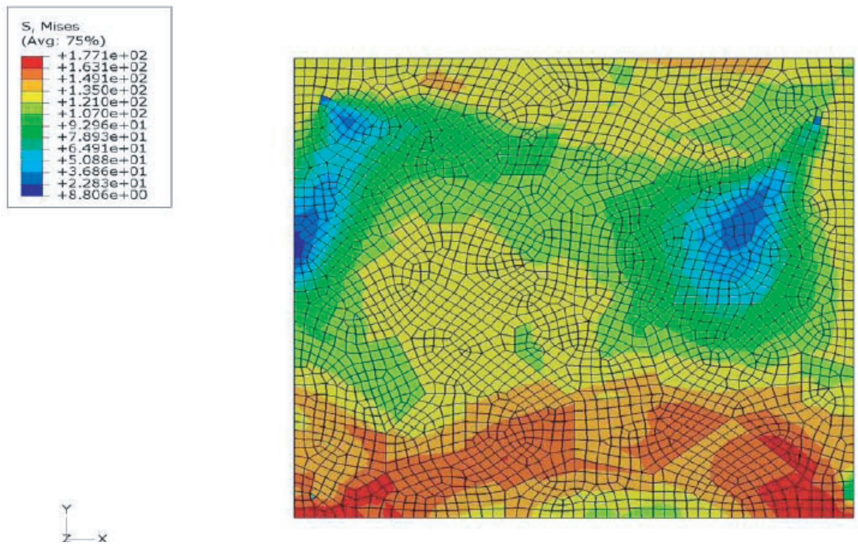

Figure 7: Equivalent stress for grain size set 1 with assign random grain orientation angle of set C after simple shear.

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