3D simulation of texture evolution induced grain coarsening in FCC polycrystals during severe plastic deformation

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Abstract. In the present work, results obtained in 3D polycrystal simulations are reported on the coalescence effect of neighbouring grains due to texture evolution. A 3D cellular automaton model was developed for this purpose, which permits to take into account the effect of topology on coalescence. The grains constituting the polycrystal were divided into voxels to have realistic representations of grain shapes. The Taylor polycrystal plasticity approach was applied to calculate the orientation change for each voxel. When the disorientation angle between neighbour voxels belonging to different grains was less than 5°, the voxel volume was reallocated to the neighbouring grain. For a random initial texture, after a shear strain of 6, the relative volume that was re-assigned between neighbours was 29.7%, which is not negligible. The effect of initial texture and topology was also investigated. The 3D morphologies of some typical coarsening grains were monitored to illustrate the simulation results.

1. Introduction
The grain refining effect during severe plastic deformation processes (SPD) is well known, and one of the major reasons why SPD is a very effective way for obtaining ultra-fine grained or even nano-structured materials [1]. However, at extreme large strains a steady state develops in the microstructure and the average grain size remains constant [2-4]. Therefore, the grain fragmentation process is balanced by a coarsening effect. It is proposed that coarsening is due to continuous dynamic recrystallization in this stage by grain boundary migration [5]. Nevertheless, a displacement of a grain boundary can be also produced as an effect of reducing the orientation difference between the two sides of the boundary. Such an effect can be produced by an evolution of the grain orientations on the two sides. If the orientations are approaching each other, the disorientation is diminishing. So by setting a minimum angle (usually 5°), if it is falling below this critical value, the grain boundary can be detected at a shifted position within the grains. Progressively, this effect is increasing the volume of one grain while reducing the neighbor’s one, so the grain size changes. Indeed, during texture evolution, grain orientations are approaching ideal positions in Euler space, and if they are neighbor grains, coalescence into one grain can take place. Such
an effect has been reported in sheet-ECAP deformation of a low carbon steel in reference [6] and was also modelled successfully in a 2D simulation. The purpose of the present study is to explore the magnitude of the coalescence effect due to texture evolution in a 3D modeling approach. The simulation work shows that the effect is not negligible; up to 30% of the sample volume can be affected by the coalescence process at sufficiently large strains.

2. Simulation procedure

2.1. Generation of a 3D polycrystal structure by cellular automaton (CA)

A 3D CA algorithm was developed to generate a 3D polycrystal aggregate. A cubic space was divided into voxels and a certain number of grain-sites were generated randomly in this space. Then the nuclei were let grow until occupying the whole space using a probability switching rule. During the growth procedure the Moore neighborhood approach was used, that considers the nearest 6 voxels and the second-nearest 12 voxels in the state switching rule. Grain IDs were assigned to each grain in order to track the grains; the voxels belonging to one grain had the same grain ID. Finally, crystallographic orientations were assigned to the grains. Periodic boundary conditions were applied to the cube for simulating an infinite system.

In this work, the polycrystal model was constructed to compose 150×150×150 voxels in the x, y, z axis directions containing 10000 grains in total. So, in average, 150×150×150 / 10000 = 338 voxels composed a grain. The voxel size was set as 1 μm ×1 μm ×1 μm. It should be noted that all grain size statistics data in the following are based on this voxel size, however, the fraction and frequency data are irrelevant to the voxel size. Figure 1(a) shows the established polycrystal geometry with a random texture generated using the ATEX software [7]. The grain size was calculated here as the diameter of a sphere having the same volume as an irregular shaped grain. The initial grain size distribution is shown in figure 1(b) in number fractions. It infers that a homogeneous equiaxed grain structure with Gaussian distribution in grain size was obtained using the developed CA model.

![3D model polycrystal and (b) its grain size distribution generated by CA.](image)

2.2. Taylor polycrystal plasticity analysis

Generally, the crystallographic texture evolution of a polycrystal during deformation needs to consider not only the orientation evolution of single grains but also the interaction between neighbor grains. Also, the grain shape would change with the progress of plastic deformation. Even for one specific grain, both the deformation and orientation evolutions are inhomogeneous within the grain, depending on its initial orientation, on the loading conditions, and also on the disorientation with its neighbors. Besides, grain fragmentation usually occurs during deformation process, resulting in a very fine microstructure after large plastic strain.
This work focuses on the texture induced grain coarsening effects during large plastic strain. Because of the good ability and efficiency for predicting orientation evolution in FCC and BCC metal polycrystals at high strain conditions [8], the full constraints Taylor model was employed in this work to simulate the orientation evolution during deformation. In this model, the interaction between neighbor grains is not considered and the voxels belonging to one grain were estimated to undergo the same changes. Nevertheless, using this approach, the effects of texture induced coarsening can be captured and the tendencies can be examined.

In the full constraints Taylor model all grains undergo the same shape change as the whole polycrystal. This means that the local velocity gradient \( g_{ij}^{(s)} \) is equal to the macroscopic one \( L_{ij} \):

\[
l_{ij}^{(s)} = L_{ij}.
\]  

The imposed deformation of a grain is obtained as the sum of independent shears in the slip systems:

\[
l_{ij}^{(s)} = \sum_{s=1}^{N} m_{ij}^{(s)} \cdot \dot{\gamma}^{s},
\]  

where \( m_{ij}^{(s)} \) is the Schmid orientation matrix of slip system indexed by \( s \), and \( \dot{\gamma}^{s} \) is the shear strain rate. The local stress-strain relation is modelled by the usual constitutive viscoplastic power law relationship between the shear rate \( \dot{\gamma}^{s} \) and the resolved shear stress \( \tau^{s} \):

\[
\tau^{s} = \tau_0 \text{sgn}(\dot{\gamma}^{s}) \left( \frac{\dot{\gamma}^{s}}{\dot{\gamma}_0} \right)^{m} = \tau_0 \left( \frac{\dot{\gamma}^{s}}{\dot{\gamma}_0} \right)^{m-1} \cdot \left( \frac{\dot{\gamma}^{s}}{\dot{\gamma}_0} \right).
\]  

Here \( m \) is the strain rate sensitivity index, \( \tau_0 \) and \( \dot{\gamma}_0 \) are the reference shear stress and reference shear rate, respectively. The resolved shear stress is related to the macroscopic stress tensor \( \sigma \) by the relation:

\[
\tau^{s} = \sigma_{ij} m_{ij}^{(s)}.
\]  

Eqs. (1-4) are the basic equations of the Taylor model with strain rate sensitivity slip to obtain the stress state of a given crystal [9]. The stress tensor provides the slip distribution, from which the orientation change of the grain can be calculated. The 12 \{111\}<110> slip systems were considered for dislocation slip. Hardening was not taken into account in the simulation. It can be justified by several arguments: i. during large strains the hardening saturates, ii. as the objective is to obtain orientation evolution, isotropic hardening would not influence it. Thus, the results obtained are valid for isotropic hardening, without actually explicitly introducing it into the simulation.

The simple shear deformation was selected for studying the grain coalescence process, by applying a macroscopic velocity gradient with the only non-zero component \( \dot{L}_{12} = \dot{\gamma} \), corresponding to shear on plane 2 in direction 1.

2.3. Grain coalescence detection and visualization

The 3D topology of the polycrystal and its orientation evolution during deformation were tracked during the simulation. A grain coalescence detection procedure was developed to count the volumes that were reallocated between neighbor grains. This was done when the disorientation angle between two voxels belonging to neighbor grains was less than 5°. After the coalescence detection process, the grain size distributions were calculated in both number-weighted and volume-weighted versions, as well as the average grain size.

For visualization of the 3D orientation data, the initial and deformed orientations of the polycrystal were output to a set of section data with positions and corresponding Euler angles. The 3D data were then analyzed by the DREAM.3D software [10]. After that, the Paraview software was used to display the generated microstructure [11]. The initial and the deformation induced textures of the polycrystal were calculated and plotted in pole figures using the ATEX software.
3. Results and discussion

Figure 2 plots the (111) pole figures (PFs) of the texture evolution during shear deformation of the polycrystal with random initial texture. The PFs present typical shear texture of FCC polycrystals, corresponding to the Taylor model used in this work. It infers that the orientations rotate near to preferred orientations very fast at the beginning of shear deformation. By increasing the shear strain, the texture becomes sharper and its maximum density increases.

![Figure 2](image)

Figure 2. Texture evolution at different shear strains of the 3D polycrystal with random initial texture. (a) initial texture, (b) texture at shear strain of 2 (c) and at shear strain of 6. (SP indicates the shear plane and the arrow is oriented in the shear direction.)

Typical morphologies of some selected grains with their orientation evolution were tracked, as shown in figure 3. The colors of the grains indicate the crystallographic orientations according to the color code. It clearly shows that with the shear strain increasing to 6, some orientations rotated to similar orientations which have similar colors. Their misorientation angles became below 5°, so they were combined to form a larger grain. Figure 3(a) and (b) shows the evolution of two initial neighbor grains while the example in figure 3(c) and (d) show that five initial neighbor grains coalesced together. The frequency of the number of coalescing grains was analyzed. It indicated that two-grain events accounted for about 60% of the coalesced volume at a shear strain of 6. With the number of coalescing grains increasing, this frequency decreased rapidly, meaning that the coalescence frequency of more than two grains into one was increasing.

The grain coalescence detection procedure was utilized to track the grain coarsening tendency during the shear deformation. The obtained results are listed in Table 1. Note that during the random initial texture assigning procedure, the misorientation angles between some neighbor voxels with different grain IDs happened to be less than 5°. This resulted in the grain number of the initial polycrystal to be 9934 instead of 10000. By increasing the shear strain, the grains rotated near to preferred orientations, forming the texture as shown in figure 2. Meanwhile, the misorientation angles between some adjacent grains decreased below 5°. Therefore, the grain number of the polycrystal decreased with increasing shear strain as listed in Table 1. The accumulated coalescing volume fraction was also calculated. It increased dramatically at the beginning and then reached a saturation state from about 4-8 shear strain. The coarsening volume fraction reached 29.7%. (A value of 17% was reported by Gu et al. in their 2D simulation for low carbon steel [6].) This means that as much as about 30% volume fraction of the polycrystal was participating in the grain coarsening effect induced by the texture evolution. Obviously, this high volume fraction cannot be ignored during large strains. The changes in average grain sizes, however, are relatively smaller, see Table 1. In number fraction, the initial average grain size of 8.48 μm increased up to 8.82 μm, while in volume fraction, from 9.00 μm to 10.38 μm.
Table 1. Grain coalescence analysis for random initial texture

| Shear strain | 0  | 1  | 2  | 4  | 6  | 8  |
|--------------|----|----|----|----|----|----|
| Grain number | 9934 | 9250 | 8763 | 8238 | 8095 | 8201 |
| Average grain size (number-weighted) (μm) | 8.48 | 8.62 | 8.72 | 8.81 | 8.84 | 8.82 |
| Average grain size (volume-weighted) (μm) | 9.00 | 9.38 | 9.76 | 10.27 | 10.45 | 10.38 |
| Coalescing volume fraction (%) | 1.4 | 13.6 | 20.9 | 27.8 | 29.7 | 28.4 |

![Initial stage](a) ![Shear strain of 6](b)

![Initial stage](c) ![Shear strain of 6](d)

Figure 3. Typical morphologies for orientation evolution induced grain coarsening events. (Note that the deformation induced grain shape change is not shown; the deformed state is shown in the initial geometry.)

The effects of the initial texture and the topology on the texture induced grain coarsening were also investigated, as shown in figure 4. A cube-type initial texture was also considered. The change in topology was simulated by changing the number of voxels. The results show that the 3D topology had relatively small influence on the grain coarsening compared to the effect of the initial texture. As can be seen in figure 4, significantly smaller volume was concerned by grain coarsening in the case of the cube initial texture. It is also apparent from figure 4 that after the coalesced volume reached a maximum, there was a decrease in the volume. This means that grain splitting could also take place, an effect which concerned grains that were initially individual, then coalesced, and finally split in orientation. See also Table 1, which shows an increase in the grain number between shears of 6 and 8. This is also an effect of texture evolution; its origin has to be looked for in the convergent/divergent nature of the rotation field in Euler space. Namely, it has been shown in Ref. [9] that in simple shear, grain orientations can cross from the convergent side of the rotation field into the divergent one. Therefore, first orientations approach each other, then, by passing the line between the convergent/divergent regions, they deviate more and more.
Figure 4. The volume fraction affected by coalescence of grains as a function of the applied shear. The effects of the initial texture and 3D topology are also shown.

4. Conclusion
The texture induced grain coarsening was analyzed at large strains in this work. For this purpose, 3D topological polycrystals were generated using a 3D cellular automaton model. The texture evolution of the polycrystal during shear deformation was calculated using the Taylor polycrystal viscoplastic approach. A grain detection analysis, based on disorientation between neighbor voxels, was employed for computing the texture induced grain coarsening effect. The observed accumulated coalescing volume fraction reached 29.7% at a shear strain of 6 for a random initial texture, together with variations in grain size. It was found that the initial texture had significant influence on the texture induced grain coarsening; the cube texture showed smaller coalescing tendency as compared to the random texture. It is concluded that the texture induced coarsening effect in SPD cannot be ignored and should be taken into account in grain refinement analyses. Therefore, the effect of texture evolution produced grain coarsening should be investigated further for different initial textures.

References
[1] Toth L S and Gu C 2014 Ultrafine-grain metals by severe plastic deformation Mater. Charact. 92 1-14
[2] Belyakov A, Sakai T, Miura H and Tsuzaki K 2001 Grain refinement in copper under large strain deformation Philos. Mag. A 81 2629-43
[3] Estrin Y and Vinogradov A 2013 Extreme grain refinement by severe plastic deformation: A wealth of challenging science Acta Mater. 61 782-817
[4] Langdon T G 2013 Twenty-five years of ultrafine-grained materials: Achieving exceptional properties through grain refinement Acta Mater. 61 7035-59
[5] Sakai T, Belyakov A, Kaibyshev R, Miura H and Jonas J J 2014 Dynamic and post-dynamic recrystallization under hot, cold and severe plastic deformation conditions Prog. Mater. Sci. 60 130-207
[6] Gu C F, Toth L S, Rusz S and Bova M 2014 Texture induced grain coarsening in severe plastic deformed low carbon steel Scripta Mater. 86 36-9
[7] Beausir B and Fundenberger J-J 2017 Analysis Tools for Electron and X-ray diffraction, ATEX-software. Université de Lorraine - Metz
[8] Suwas S and Ray R K 2014 Crystallographic texture of materials (UK: Springer)
[9] Toth L S, Gilormini P and Jonas J J 1988 Effect of rate sensitivity on the stability of torsion textures Acta Metall. 36 3077-91
[10] Groeber M A and Jackson M A 2014 DREAM.3D: A Digital Representation Environment for the Analysis of Microstructure in 3D Integrating Mater. Manuf. Innovation 3 56-72
[11] Ayachit and Utkarsh 2015 The paraview guide: a parallel visualization application (Kitware: ISBN 978-1930934306)