Comparison of lamellar nanostructured cubical and spherical statistical volume elements in terms of crystallographic texture and deformation behaviour

Srihari Dodla

1Department of Mechanical Engineering, SRM Institute of Science and Technology, Kattankulathur, Chennai, India.

E-mail: srihariovgu@gmail.com

Abstract. This study presents the numerical homogenization of spherical and cubical statistical volume element (SVE). Numerical homogenization with periodic boundary conditions for spherical and cubical SVEs has been employed. The lamellar structure of eutectic Copper (Cu)-Silver (Ag) has been focused for the investigation of deformation behaviour and texture evolution. The initial texture for cold-drawn eutectic Cu-Ag composite has been approximated by a set of 200 discrete orientations. The comparison of deformation behaviour and the crystallographic texture has been investigated for two different SVEs. It is demonstrated that the SVEs with cubical shape induce an anisotropy when compared with the spherical SVEs. The numerical results for cubical and spherical SVEs in terms of deformation behaviour and crystallographic texture are in good agreement with the experimental observations.

1. Introduction

Materials with microstructure can have an effect on the mechanical properties on the macroscale. For example, polycrystalline materials exhibit crystallographic orientation and grain morphology. By using the numerical homogenization, the effective material properties can be calculated considering the information (arrangement and the properties) of individual constituents at a lower scale.

In order to identify the mechanical properties, different homogenization methods are at hand. For example, Klusemann and Svendsen [1] compared the homogenization methods for elastic properties. Fritzen et al. [2] investigated the effective material response for spherical porous materials. However, the analytical homogenization methods are limited in many cases such as texture evolution. Finite element methods with the periodic boundary conditions are the practical approach to understand the grain morphology and to extract the induced anisotropy present in the material.

In general, the numerical homogenization methods by RVE or SVE approach are quite popular. In these approaches (RVE or SVE), a section of the representative material is considered and the appropriate boundary conditions are defined. It can be solved either by initial- value or boundary-value problem by choosing the finite element numerical methods. With this approach, one can determine the dependent variables by volume averaging, or analyse the different microstructural effects on the effective mechanical behavior [3]. In general, the RVE itself should be representative and several studies have shown that the RVE depends on the material under consideration [4, 5, 6].

1 To whom any correspondence should be addressed.
In the current work, we study the effect of the SVE (cubical and spherical) on the macroscopic stress-strain behavior. In the case of finite element numerical homogenization, the cubical SVE is quite popular. We present the spherical SVE along with the cubical SVE. In general, the spherical SVE is advantageous because of lower surface-to-volume ratio in comparison with cubical SVE. In addition, the RVEs with spherical shape do not make a material-independent anisotropy. In the case of cubical RVEs, material-independent anisotropy is quite common with periodic boundary conditions.

The article is integrated as follows. Microstructure and the initial texture of Cu-Ag polycrystal are introduced in section 2. The elasto-viscoplastic material model has been presented in section 3. In section 4, the finite element simulations of cubical and spherical SVEs are presented. Section 5 shows the results in terms of mechanical behavior and the crystallographic texture and gives summary.

Figure 1. Microstructure of two-phase lamellar Cu-Ag composite in transverse direction (TD).

2. Initial texture
In this study, we consider a metal formed (cold-drawn) Cu-Ag polycrystal (more details about the experimental investigations of Cu-Ag rod are given in [7, 8]). Figure 1 shows the microstructure of Cu-Ag rod in the transverse direction showing the combination of grains and lamellar Cu/Ag regions. By using the X-ray analysis, the XRD measurements are performed at centre location of the Cu-Ag rod. The measured texture has been approximated by 200 grains and the texture is given as (110) pole figure. Figure 2 represents measured and approximated texture of phases (Cu and Ag) for Cu-Ag cold-drawn rod.

Figure 2. (a) and (b) Measured pole figures (110) for Cu phase and Ag phase, (c) and (d) approximated pole figures (110) by 200 orientations for Cu phase and Ag phase.

3. Material model
3.1. Constitutive law
An elasto-viscoplastic single crystal material model has been applied for the Cu and Ag phases with lamellar structure. For details see, e.g., [9, 10, 11].
The elastic reference law can be expressed as
where \( K \) is the fourth order constant stiffness tensor. The 2nd Piola-Kirchhoff stress \( T^{2PK} \) in linear relation with the Cauchy-Green strain tensor.

3.2. Flow rule
Using the slip systems of single crystal, the flow rule is given as

\[
F_p F_p^{-1} = \sum_\alpha \dot{\gamma}^\alpha \tilde{d}_\alpha \otimes \tilde{n}^\alpha
\]

where \( F_p \) is the plastic part of \( F \). For each slip system \( \alpha \), the slip direction is \( \tilde{d}_\alpha \) and the slip plane normal is \( \tilde{n}_\alpha \) in the isoclinic placement. The rate of plastic shear strain \( \gamma^\alpha \) for each slip system has been suggested by Hutchinson [12] in the form of

\[
\dot{\gamma}^\alpha = \dot{\gamma}_0 \text{sgn}(\tau^\alpha) \left| \frac{\tau^\alpha}{\tau^\alpha_c(\gamma)} \right|^m
\]

In Eq. (3), \( m \) and \( \gamma_0 \) are the strain rate sensitivity parameter and the constant reference shear rate. Both \( \gamma_0 \) and \( m \) are considered as material constants. \( \tau^\alpha_c \) is the resolved shear stress. It can be obtained as

\[
\tau^\alpha_c := \tilde{C} \tilde{T}^{2PK} : \tilde{d}_\alpha \otimes \tilde{n}^\alpha
\]

where the upper tilde shows that the tensors are defined in the isoclinic reference placement.

3.3. Hardening rule
The hardening law is given by Voce [13], has been considered to calculate the strain hardening rate as a function of the shear stress.

\[
\dot{\tau}^\alpha_c = \tau_{c0} + (\tau_s + \theta_\infty \gamma)(1 - \exp(-\theta_0 \gamma/\tau_s))
\]

where \( \tau_{c0}, \tau_s, \theta_\infty, \theta_0 \) are hardening parameters.

The shear strain \( \gamma \) is given as

\[
\gamma = \int \sum_\alpha |\gamma_\alpha| \, dt
\]

The following hardening law [14] is used for the evolution of hardening in the multiple slip case

\[
\dot{\tau}^\alpha_c = \sum_\beta h_{\alpha\beta} \dot{\gamma}^\beta, \quad h_{\alpha\beta} = q_{\alpha\beta} \theta(\gamma)
\]

where \( \dot{\tau}^\alpha_c \) is the rate of critical resolved shear stress, \( \dot{\gamma}^\beta \) is given as the shear strain rate of all slip systems, \( \theta(\gamma) = \frac{\partial \gamma^\alpha}{\partial \gamma} \) is the rate of single slip hardening, \( q_{\alpha\beta} \) is the matrix combining the self and latent hardening.
4. Statistical volume element (SVE)

By the help of the finite element software ABAQUS [15] the calculations have been carried out. Poisson-Voronoi microstructure [16, 10] has been created inside the SVE (cubical and spherical) with periodic boundary conditions. In this paper, the measured texture has been approximated by 200 grains, these 200 grains have been considered to investigate the deformation process. In particular, the numerical predictions (uniaxial compression) with the mechanical behavior and the texture evolution are studied in Cu-Ag polycrystal. The cubical SVE of the Cu-Ag polycrystal with 200 grains is depicted in figure 3. Figure 3 (A) shows the cubical SVE with 200 grains and the figure 3 (B) presents the alternate layers of lamellae (Cu, Ag) in the grains.
Figure 4 shows the spherical SVE of the lamellar structure (Cu and Ag) with 200 grains. Figure 4 (A) represents the grains with periodic boundary conditions. Each color corresponds to a different grain orientation. The lamellar structure (Cu and Ag) inside the grains are displayed in figure 4 (B).

![Figure 4](image)

**Figure 4.** Shows the spherical SVE of the lamellar structure (Cu and Ag) with 200 grains. Figure 4 (A) represents the grains with periodic boundary conditions. Each color corresponds to a different grain orientation. The lamellar structure (Cu and Ag) inside the grains are displayed in figure 4 (B).

5. Simulated results

The numerical results in terms of stress-strain response and the texture (pole figures and the orientation distribution function) for the cubical and spherical SVEs are presented. The experimental measured and validated mechanical behavior in simple compression of cubical SVE with 200 grains are depicted in figure 5. The simulated mechanical behavior of cubical SVE is in good agreement with the experimental behavior. The simulated stress-strain behavior of spherical SVE with 200 grains and the experimental measured one are shown in figure 6. As seen in figure 6, the stress-strain behavior of spherical SVE is identical with respect to the experimental results.

![Figure 5](image)

**Figure 5.** Comparison of stress-strain curves of uniaxial compression for cubical SVE.

![Figure 6](image)

**Figure 6.** Comparison of stress-strain curves of uniaxial compression for spherical SVE.

![Figure 7](image)

**Figure 7.** Pole figures: (A and D) Measured Cu and Ag phase, (B and E) Simulated Cu and Ag phase for cubical SVE, and (C and F) simulated Cu and Ag phase for spherical SVE.
Figure 8. ODF for Cu phase: (A) measured, (B) simulated for cubical SVE, and (C) simulated for spherical SVE.

Figure 9. ODF for Ag phase: (A) measured, (B) simulated for cubical SVE, and (C) simulated for spherical SVE.
The crystallographic texture is depicted in terms of the pole figure and the orientation distribution function (ODF). Fig. 7 represents the measured and simulated pole figure of Cu and Ag phases after compression testing. Fig. 7 (A and D) presents the measured pole figure of Cu and Ag phases after compression testing. Fig. 7 (B and E) represents the simulated pole figure for Cu and Ag phases for cubic SVE. Similarly, Fig. 7 (C and F) is shown for the spherical SVE. ODF is given in the space of Bunge Euler angles \((\phi_1 \leq 90^\circ, \phi \leq 90^\circ)\), \(\phi_2(= 0^\circ, 45^\circ, 65^\circ)\), it has been presented in figure 8 and 9. The simulated ODF for the cubical and spherical SVE is compared with the measured ODF for both phases (Cu and Ag) in figure 8 and 9. From the texture plots, it is observed that the alloy type texture for the Cu and Ag phases. The simulated texture results are in good agreement with the measured ODF data. In the ODF plot (see figure 8 and 9), the texture components are depicted and the important components observed are Brass, Copper, Goss and S.

6. Conclusion
The performance of the cubical and spherical SVE are compared with periodic boundary conditions for a Cu-Ag polycrystal. From the numerical investigations, it is observed that the cubical and spherical SVEs are capable of implementing 200 grains along with a lamellar structure of Cu and Ag. The material behavior of Cu and Ag phase at each integration point is given by using the elasto-viscoplastic material model at microscale. The developed numerical models (cubical and spherical) are able to simulate the crystallographic texture of each phase. The simulated ODF for both phases is in good agreement with the measured ODF. Four different texture components such as Brass, Copper, Goss and S are captured.

7. References
[1] B Klusemann and B Svendsen 2010 Homogenization methods for multi-phase elastic composites: Comparisons and benchmarks Technische Mechanik 30 374–386
[2] F Fritz, S Forest, T Bohlke, D Kondo and T Kanit 2012 Computational homogenization of elasto-plastic porous metals International Journal of Plasticity 29 102–119
[3] R Glu¨ge, M Weber and A Bertram 2012 Comparison of spherical and cubical statistical volume elements with respect to convergence, anisotropy and localization behavior Computational Materials Science 63 91–104
[4] T Kanit, S Forest, I Galliet, V Mounoury and D Jeulin 2003 Determination of the size of the representative volume element for random composites: statistical and numerical approach International Journal of Solids and Structures 40 3647–3679
[5] A Salahouellahj and H Haddadi 2010 Estimation of the size of the RVE for isotropic copper polycrystals by using elastic-plastic finite element homogenisation Computational Materials Science 48 447–455
[6] XF Xu and X Chen 2009 Stochastic Homogenisation of Random Elastic Multi-Phase Composites and Size Quantification of Representative volume element. Mechanics of materials 41 174 – 186
[7] S Dodla, P Thiem, M Kru´ger, D Dietrich and A Bertram 2015 Microstructure, flow behavior, and bulk texture evolution of cold drawn copper-silver composites Journal of Alloys and Compounds 647 519–527
[8] Dodla Srihari 2015 Experimental Investigations and Numerical Simulations of Lamellar Cu-Ag Composites docupoint 16
[9] A.Bertram 2012 Elasticity and Plasticity of Large Deformations - an Introduction third edition springer
[10] Srihari Dodla, A Bertram and M Krueger 2015 Finite element simulation of lamellar copper-silver composites Computational Materials Science 101 29–38
[11] S Dodla and A Bertram 2016 Numerical Study of the Deformation Behavior of Eutectic Cu/Ag Polycrystals Technische Mechanik. 36(3) 155–165
[12] J Hutchinson 1976 Bounds and self-consistent estimates for creep of polycrystalline materials. *Proc. R. Soc.* **348** 101–127
[13] E Voce A practical strain-hardening function *Metallurgia* **51** 219–226
[14] R Hill 1966 Generalized constitutive relations for incremental deformation of metal crystals by multislip *Journal of the Mechanics and Physics of Solids* **14** 95–102
[15] Hibbitt, Karlsson and Sorensen 1990 *ABAQUS Reference Manuals* Addison-Wesley
[16] S Kumar and S K Kurtz 1994 Simulation of material microstructure using a 3D Voronoi tesselation: Calculation of effective thermal expansion coefficient of polycrystalline materials *Acta Metallurgica et Materialia* **42** 3917–3927