

**Task 1. Tensile properties (20 points, Lecture3)**

**1.1** For a bronze alloy, the stress at which plastic deformation begins is 271 MPa and the modulus of elasticity is 150 GPa. (a) What is the maximum load that may be applied to a specimen having a cross-sectional area of 270 mm<sup>2</sup> without plastic deformation? (b) If the original specimen length is 123 mm, what is the maximum length to which it may be stretched without causing plastic deformation? (Please give the detailed calculation process.)

**Solution:**

**(a)** The maximum load applied without plastic deformation should be:

$$F = \sigma_{\text{yield}} \cdot A_0 = 271 \text{ MPa} \cdot 270 \text{ mm}^2 = 73.17 \text{ kN} \text{ (2 points)}$$

**(b)** In the elastic deformation region, the stress-strain relationship obeys Hook's Law:

$$\sigma_{\text{yield}} = E \cdot \varepsilon_e \quad \text{Eq. 1}$$

$E$  is the Young's modulus of elasticity.

The plastic deformation begins is 271 MPa, so the maximum strain without plastic deformation should be:

$$\varepsilon_e = \frac{\sigma_{\text{yield}}}{E} = \frac{271 \text{ MPa}}{150 \text{ GPa}} \approx 1.81 \times 10^{-3} \text{ (2 points)}$$

According to the strain definition:

$$\varepsilon_e = \frac{\Delta l}{l_0} = \frac{l_e - l_0}{l_0} = \frac{l_e}{l_0} - 1 \quad \text{Eq. 2 (1 point)}$$

$$\text{we will have: } \frac{l_e}{l_0} = \varepsilon_e + 1 = 1.00181 \text{ (1 point)}$$

$$l_e = 1.00181 \cdot l_0 = 1.00181 \times 123 \text{ mm} \approx 123.22 \text{ mm} \text{ (1 point)}$$

**1.2** Consider the brass alloy the stress-strain behavior of which is shown in Figure1. A cylindrical specimen of this alloy 14 mm in diameter and 173 mm long is to be pulled in tension. Calculate the force necessary to cause a 0.0087 mm reduction in diameter. Assume a value of 0.33 for Poisson's ratio. (Please give the detailed calculation process.)

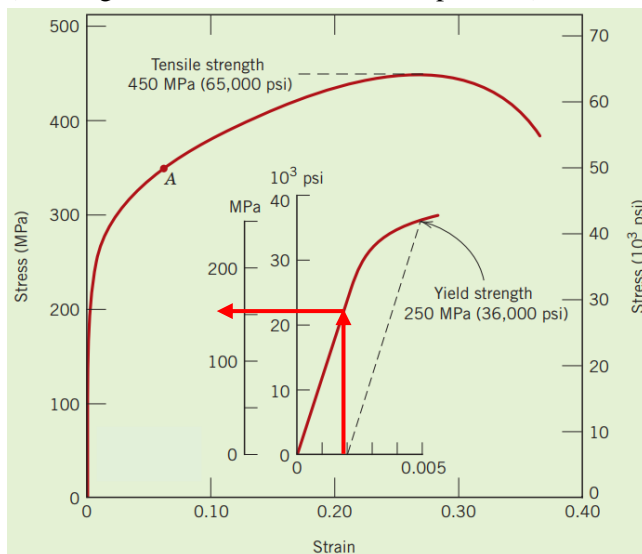


Figure 1 The stress-strain curve of a brass alloy. [1]

**Solution:**

$D_0 = 14 \text{ mm}$ ,  $\Delta D = 0.0087 \text{ mm}$ , we can derive strain in diametrical direction:

$$\varepsilon_x = -\frac{\Delta D}{D_0} = -\frac{0.0087 \text{ mm}}{14 \text{ mm}} \approx -6.21 \times 10^{-4} \text{ (1 point)}$$

According to Poisson's ratio definition:

$$\nu = -\frac{\varepsilon_x}{\varepsilon_z} = -\frac{-6.21 \times 10^{-4}}{\varepsilon_z} = 0.33 \text{ (1 point)}, \text{ so } \varepsilon_z = \frac{-6.21 \times 10^{-4}}{0.33} = 0.0019 \text{ (1 point)}$$

According to Figure 1, we can read the stress value (as marked with red arrows):

$$\sigma_z \approx 150 \text{ MPa (1 point)}$$

(Here  $\varepsilon_z = 0.0019$  is the elastic strain, the corresponding stress is read with the perpendicular line to the strain axis)

So the necessary force can be derived by:

$$F = \sigma_z \cdot A_z = \sigma_z \cdot \pi \cdot \frac{(D_0)^2}{4} = 150 \text{ MPa} \times \pi \times \frac{(14 \text{ mm})^2}{4} = 23.09 \text{ kN (2 points)}$$

**1.3** Prove the validity of the following equation for the end of the uniform elongation in tensile tests (Considère-construction): (Give the derivation process)

$$\frac{d\sigma_T}{d\varepsilon} = \frac{\sigma_T}{1 + \varepsilon}$$

Where  $\sigma_T$  is the true stress;  $\varepsilon$  is the engineering strain.

**Solution:**

According to the definition of true stress:

$$\sigma_T = F/A \quad \text{Eq. 3}$$

where  $F$  is the force,  $A$  is the instantaneous cross-section area.

Therefore,

$$F = \sigma_T \cdot A \quad \text{Eq. 4 (1 point)}$$

The ultimate tensile strength (UTS) is defined as the maximum engineering strength, i.e. maximum forces instance, with the uniform elongation. Hence, at the UTS moment,

$$dF = 0 = A \cdot d\sigma_T + \sigma_T \cdot dA \quad \text{Eq. 5 (1 point)}$$

and

$$\frac{dA}{A} = -\frac{d\sigma_T}{\sigma_T} \quad \text{Eq. 6 (1 point)}$$

Because of the constant volume during plastic deformation, we will have:

$$l_0 \cdot A_0 = l \cdot A = \text{constant} \quad \text{Eq. 7 (1 point)}$$

$$\frac{dl}{l} = -\frac{dA}{A} = \frac{d\sigma_T}{\sigma_T} \quad \text{Eq. 8 (1 point)}$$

where  $l_0$  and  $A_0$  are the initial length and cross-section areas, respectively, and  $l$  is the instantaneous length.

In addition, according to the definition of true strain and engineering strain, the relation between true strain  $\varepsilon_T$  and engineering strain  $\varepsilon$  is:

$$\varepsilon_T = \int_{l_0}^l \frac{dl}{l} = \ln \frac{l}{l_0} = \ln \frac{l_0 + \Delta l}{l_0} = \ln(1 + \varepsilon) \quad \text{Eq. 9 (1 point)}$$

(Please notice the difference between definite integral and indefinite integral. If you don't give the upper and lower bounds of the integral, you won't get an exact integral value.)

Therefore,

$$\frac{dl}{l} = d\varepsilon_T = \frac{d\varepsilon}{1 + \varepsilon} \quad \text{Eq. 10 (1 point)}$$

Combine Eq. 8 and Eq. 10:

$$\frac{d\sigma_T}{d\varepsilon} = \frac{\sigma_T}{1 + \varepsilon} \quad \text{Eq. 11}$$

## Task 2. Plastic deformation and strength (55 points, Lecture4)

**2.1** Name and explain three important possibilities for increasing the strength of pure metals and alloys. (9 points)

### Solution:

Three important strengthening mechanisms are:

- Grain refinement

Because grain boundaries can act as barriers to dislocation motion, so the finer average grain size in materials, the higher yielding stress is. It obeys Hall-Petch relationship equation:

$$\sigma_{yield} = \sigma_0 + k_y \cdot d^{-\frac{1}{2}} \quad \text{Eq. 12}$$

Herein,  $\sigma_0, k_y$  are material constants.

- Solid solution strengthening

The technique works by adding atoms of one element (the alloying element) to the crystalline lattice of another element (the base metal), forming a solid solution. The local non-uniformity in the lattice due to the alloying element makes plastic deformation more difficult by impeding dislocation motion through stress fields. In contrast, alloying beyond the solubility limit can form a second phase, leading to strengthening via other mechanism (e.g. the precipitation of intermetallic compounds).

- Strain hardening

Strain hardening (or cold working) is the strengthening of most metals by plastic deformation at room temperature. This strengthening occurs because of dislocation movements and dislocation generation within the crystal structure of the material. Alloys not amenable to heat treatment, including low-carbon steel, are often strain-hardened. Some alloys can only be strengthened via this, such as pure copper and aluminum.

(3 points for each mechanism)

**2.2 (a)** List, individually, the most possible slip systems in the fcc and bcc metals (Hint: 12 independent slip systems for each structure, ignoring the repeated inverse planes, e.g. (111) and  $(\bar{1}\bar{1}\bar{1})$  are the same plane, only (111) shall be taken into account). (24 points)

(b) Derive the Schmid law based on the schematic drawing of a single crystal under tensile loading (Figure 2), and define the Schmid factor. (5 points)

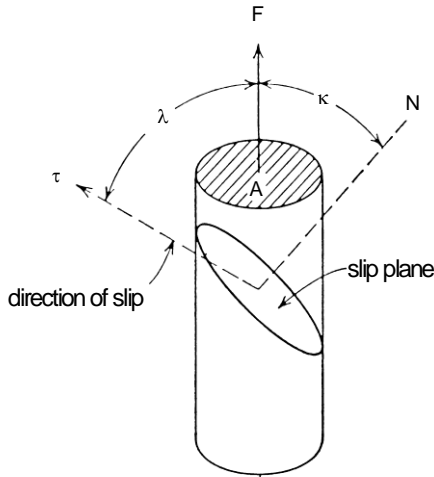


Figure 2 Schematic diagram of Schmid law. [2]

(c) The axis of a tensile specimen of an **fcc** Fe single crystal is parallel to the  $[\bar{1}25]$ -direction, based on the possible slip systems defined in Task2.2 (a), calculate the Schmid factor for every slip system. (Please give the detailed calculation process for at least one individual slip system.) (13 points)

(d) In terms of the case in Task2.2 (c), among all these 12 slip systems, which one will be activated first? Why? If the critical resolved shear stress is 2.7 MPa, for plastic deformation, which tensile stress has to be applied (in MPa)? (Please give the detailed calculation process.) (4 points)

**Solution:**

**(a):** See Table 1.

Table 1 Most important slip systems of BCC and FCC.

| BCC                      | FCC                      | Schmid factor for 2.2(c) |
|--------------------------|--------------------------|--------------------------|
| $(110)[\bar{1}11]$       | $(111)[1\bar{1}0]$       | -0.2449                  |
| $(110)[1\bar{1}1]$       | $(111)[10\bar{1}]$       | -0.4899                  |
| $(1\bar{1}0)[111]$       | $(111)[01\bar{1}]$       | -0.2449                  |
| $(1\bar{1}0)[11\bar{1}]$ | $(\bar{1}11)[110]$       | 0.1089                   |
| $(101)[\bar{1}11]$       | $(\bar{1}11)[101]$       | 0.4355                   |
| $(101)[11\bar{1}]$       | $(\bar{1}11)[01\bar{1}]$ | -0.3266                  |
| $(10\bar{1})[111]$       | $(1\bar{1}1)[110]$       | 0.0272                   |
| $(10\bar{1})[1\bar{1}1]$ | $(1\bar{1}1)[10\bar{1}]$ | -0.1633                  |
| $(011)[1\bar{1}1]$       | $(1\bar{1}1)[011]$       | 0.1905                   |
| $(011)[11\bar{1}]$       | $(11\bar{1})[1\bar{1}0]$ | 0.1633                   |
| $(0\bar{1}1)[111]$       | $(11\bar{1})[101]$       | -0.2177                  |
| $(0\bar{1}1)[\bar{1}11]$ | $(11\bar{1})[011]$       | -0.3810                  |

(24 points in total; if you use the wrong Miller indices/Slip system symbol, -2 points)

**(b):**

First, here are some definitions in Figure 2:

A – the cross-section area of the single crystal,

A' – the area of the slip plane,

F – external loading force,

$F'$  – the resolved force along the slip direction on the slip plane.

$\lambda$  - angle between the external loading axis and the slip direction,

$\kappa$  - angle between the external loading axis and the slip plane normal direction,

Therefore, the resolved shear stress is:

$$\tau = \frac{F'}{A'} \quad \text{Eq. 13 (1 point)}$$

Based on the geometry relationship shown in Figure 2, we can have:

$$F' = F \cdot \cos \lambda \quad \text{Eq. 14 (1 point)}$$

$$A' = A / \cos \kappa \quad \text{Eq. 15 (1 point)}$$

Combine the above equations, we will get:

$$\tau = \frac{F'}{A'} = \frac{F \cdot \cos \lambda}{A / \cos \kappa} = \sigma \cdot \cos \lambda \cdot \cos \kappa \quad \text{Eq. 16 (1 point)}$$

where  $\sigma$  is the tensile stress, and  $m = \cos \lambda \cdot \cos \kappa$  is called as the Schmid factor (1 point). For tensile deformation, it is assumed that  $0 < |m| < 0.5$ . The acting force on a dislocation depends on the orientation of the slip system relative to the tensile axis. If there is more than one slip system in a crystal structure, the different slip systems usually have different Schmid-factors. For a given tensile stress the slip system with the largest Schmid-factor experiences the highest shear stress. Dislocation motion sets in if the force on the dislocation and, correspondingly, the resolved shear stress exceeds a critical value, i.e. the critical resolved shear stress  $\tau_{crit}$ . This critical shear stress should be the same for all slip systems. This is the statement of Schmid's law. Experiments do confirm this hypothesis. [2]

**(c):**

The angle  $\theta$  between two vectors  $\vec{a}$ ,  $\vec{b}$  and be calculated according to:

$$\cos \theta = \frac{\vec{a} \cdot \vec{b}}{|\vec{a}| |\vec{b}|} \quad \text{Eq. 17}$$

The force axis direction is  $[\bar{1}23]$ , take the first FCC slip system  $(111)[1\bar{1}0]$  in Table 1 as an example, its Schmid factor is:

$$m = \cos \lambda \cdot \cos \kappa = \frac{((-1) \times 1 + 2 \times (-1) + 5 \times 0)}{\sqrt{(-1)^2 + 2^2 + 5^2} \cdot \sqrt{1^2 + (-1)^2 + 0^2}} \cdot \frac{((-1) \times 1 + 2 \times 1 + 5 \times 1)}{\sqrt{(-1)^2 + 2^2 + 5^2} \cdot \sqrt{1^2 + 1^2 + 1^2}} = -0.2449 \quad (1 \text{ point})$$

The same calculation can be done for other slip systems. The results are summarized in Table 1. (12 points)

**(d):**

The  $(111)[10\bar{1}]$  slip system will be active first, as it has the maximum absolute Schmid factor. (1 point for slip system, 1 point for explanation)

Therefore, the required tensile stress is:

$$\sigma = \frac{\tau}{|\cos \lambda \cdot \cos \kappa|} = \frac{2.7 \text{ MPa}}{0.4899} = 5.5114 \text{ MPa} \quad (2 \text{ points})$$

### Task 3. Representative volume element (25 points, Exercise2)

(a) Explain what the representative volume element (RVE) is.

(b) Generate two RVEs with the following common parameters and different phase fraction values:

|                    | Phase 1         | Phase 2 | × | Phase 1 | Phase 2 |
|--------------------|-----------------|---------|---|---------|---------|
| Grain size, mu     | 3               | 2       |   | 0.3     | 0.7     |
| Grain size, sigma  | 0.5             | 0.5     |   |         |         |
| Grain shape, alpha | 15              | 5       |   |         |         |
| Grain shape, beta  | 1.5             | 30      |   | 0.7     | 0.3     |
| Dimensions         | (100, 100, 100) |         |   |         |         |
| Resolution         | (2, 2, 2)       |         |   |         |         |
| Origin             | (0, 0, 0)       |         |   |         |         |

(Hint: Generate RVEs with Dream.3D then plot them with ParaView. Please plot both grain and phase maps for the generated RVEs with legends. You can also use the threshold to display each phase. You can use the EulerAngles or IPFcolors as color coding for better presentation of the grain structure.)

#### Solution:

**(a): (5 points)**

There are several definitions and explains of the representative volume element (RVE) in literatures:

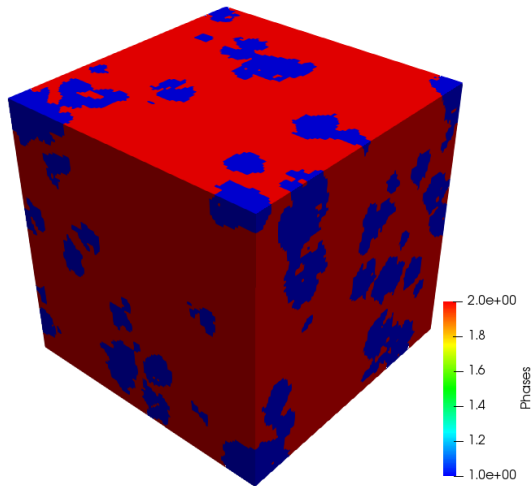
- An RVE is the minimal material volume, which contains enough statistically mechanisms of deformation processes. The increasing of this volume should not lead to changes of evolution equations for field-values and mechanisms descriptions [3].
- The RVE must be chosen “sufficiently large” compared to the microstructural size for the approach to be valid. The RVE is the smallest material volume element of the composite for which the usual spatially constant “overall modulus” macroscopic constitutive representation is a sufficiently accurate model to represent mean constitutive [4].
- The RVE is a model of the material to be used to determine the corresponding effective properties for the homogenized macroscopic model. The RVE should be large enough to contain sufficient information about the microstructure in order to be representative, however, it should be much smaller than the macroscopic body. This is known as the Micro-Meso-Macro principle [5].
- The RVE is defined as the minimum volume of laboratory scale specimen, such that the results obtained from this specimen can still be regarded as representative for a continuum [6].
- The RVE is very clearly defined in two situations only: i) unit cell in a periodic microstructure, and ii) volume containing a very large (mathematically infinite) set of microscale elements (e.g. grains), possessing statistically homogeneous and ergodic properties [7].

To sum up, the RVE is usually regarded as a sub-volume of the heterogeneous material that is sufficiently large to be statistically representative of the microstructural heterogeneities, i.e., grains, inclusions, voids, fibers, etc. This is generally the principle adopted, and it leads to the fact that the RVE must include a large number of the composite micro-heterogeneities and provide necessary statistical information about the material. It must however remain small enough to be considered as a volume element of continuum mechanism.

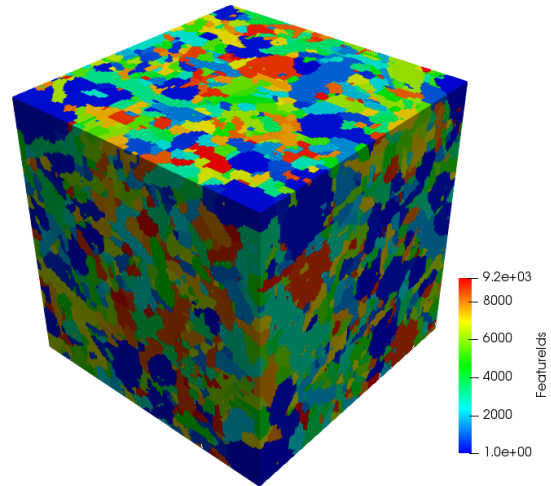
**(b): (20 points)**

The operation steps are introduced in Exercise02 slides. The generated RVEs are shown in Figure 3 and Figure 4.

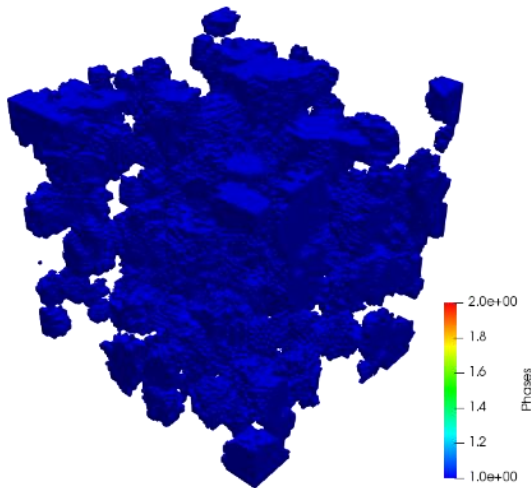




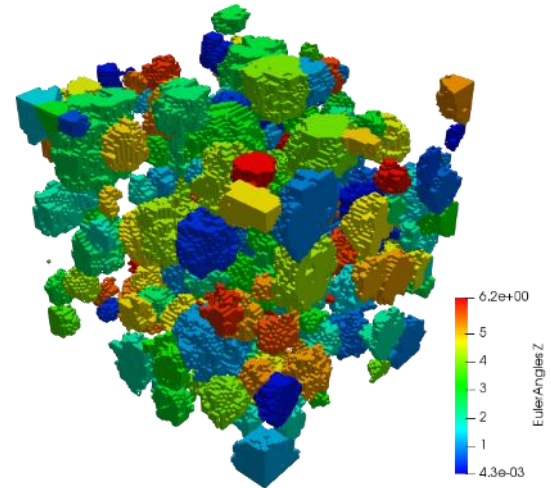
(a) Phase map of RVE1 (3 points)



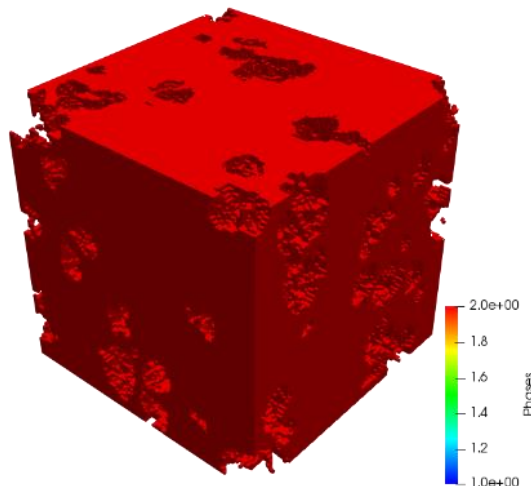
(b) Grain map of RVE1, coloring by grain ID (3 points)



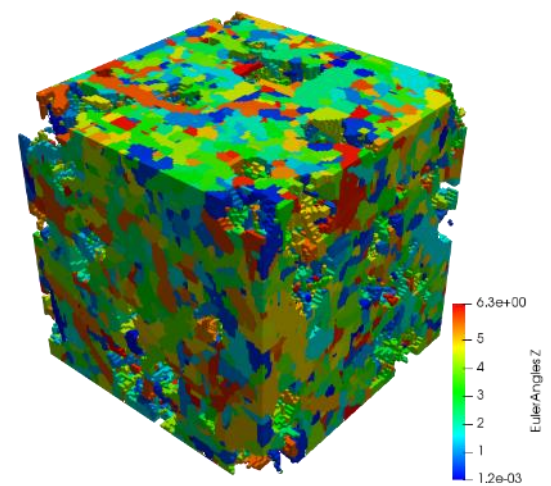
(c) Phase map of RVE1 - phase1 (1 point)



(d) Grain map of RVE1 - phase1, coloring by EulerAngles-X (1 point)

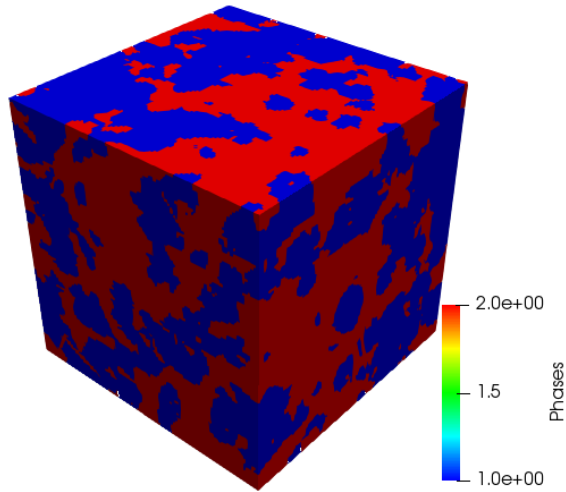


(e) Phase map of RVE1 - phase2 (1 point)

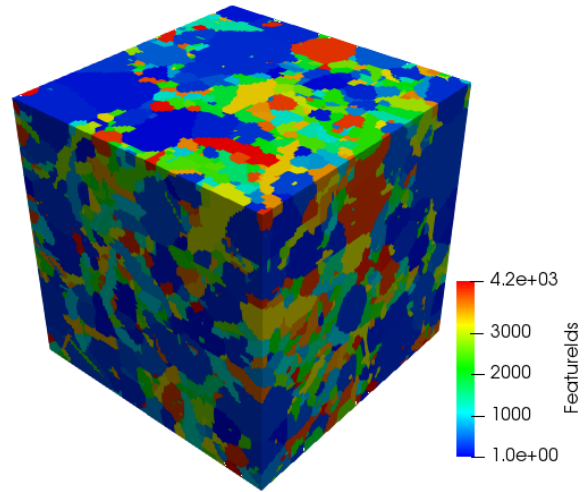


(f) Grain map of RVE1 - phase2, coloring by EulerAngles-X (1 point)

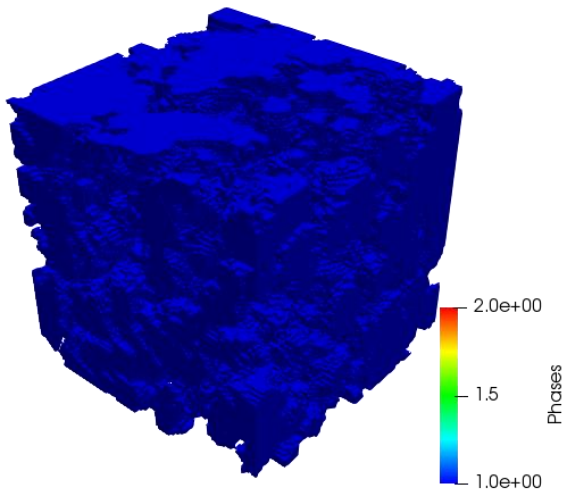
Figure 3 The generated RVE1 with 30 % phase1 and 70% phase2.



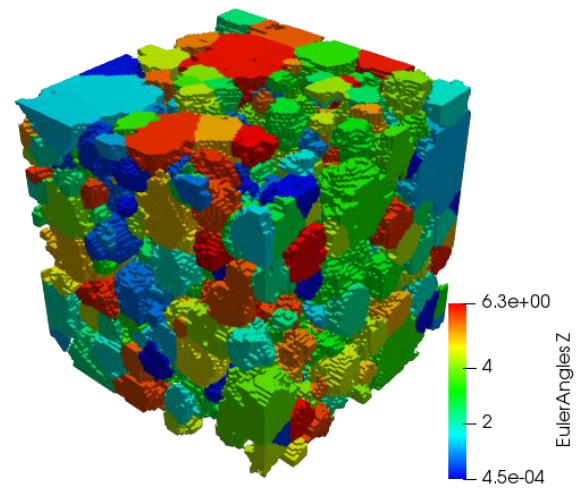
(a) Phase map of RVE2 (3 points)



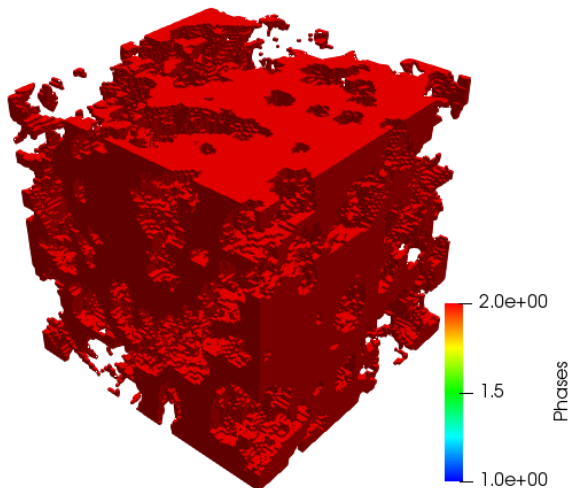
(b) Grain map of RVE2, coloring by grain ID (3 points)



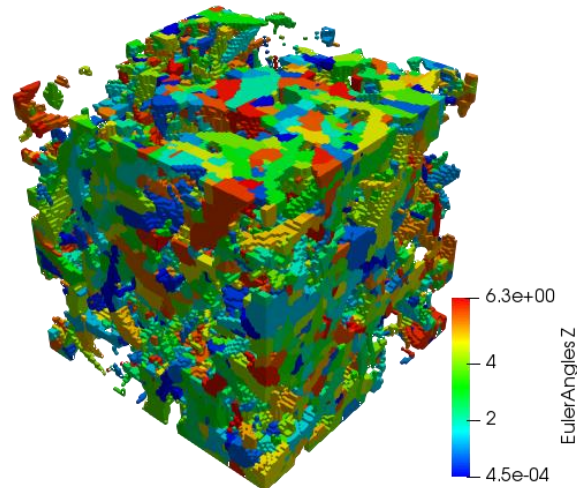
(c) Phase map of RVE2 - phase1 (1 point)



(d) Grain map of RVE2 - phase1, coloring by EulerAngles-X (1 point)



(e) Phase map of RVE2 - phase2 (1 point)



(f) Grain map of RVE2 - phase2, coloring by EulerAngles-X (1 point)

Figure 4 The generated RVE2 with 70% phase1 and 30% phase2.



**Reference:**

- [1] W. D. Callister and D. G. Rethwisch, *Materials Science and Engineering: An Introduction*, 8th Edition, Wiley, 2009.
- [2] G. Gottstein, *Physical Foundations of Materials Science*, Springer-Verlag Berlin Heidelberg, Berlin, Germany, 2004.
- [3] P.V. Trusov, I.E. Keller, Theory of constitutive relation: Part I. Perm Russian: Perm State Technical University, 1997.
- [4] W.J. Drugan, J.R. Willis, J. Mech. Phys. Solids, 44 (1996) 497–524.
- [5] Z. Hashin, Journal of Applied Mechanics, 50 (1983) 481–505.
- [6] J.G.M. van Mier. Fracture processes of concrete. USA: CRC Press, Inc., 1997.
- [7] M. Ostoja-Starzewski, The use, misuse, and abuse of stochastics in mechanics of random media. In Z. Waszczyszyn and J. Pamin, editors, Eur. Conf. Comp. Mech., 2001.

**Due date: 18:00, 14.11.2021.**

**Contact: MyCourses ‘General discussion’ channel,**

**Q&A: every Tuesday at 16:30-18:00 (via Zoom: <https://aalto.zoom.us/j/62428835336> ).**