

# COE-C2004 - Materials Science and Engineering

# Exercise 6

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## **Outline**

- Important announcements
- Feedback on Assignment 5
- Case study
- Exam
- Feedback & Questions



## Important updates

Lectures:

Week 6 (Dec 6 – 12)

- L12-Video online: Review lecture
- No lectures on Dec 6 & 10
- Final Exercise/Q&A: Dec 9
- The grading weight of assignment will be accordingly modified.
  - A1-A3, 8 points
  - A4-A5, 5 points
  - A6, 6 points, opening on Dec 07.
  - In total, 40 points for 6 assignments. Your final grades will be accordingly updated in MyCourses system.
- The case study has been opened in MyCourses. Additional points => Total grade in MyCourses is not correct.
- For A6 (DDL: 18:00 12.12.2021), no extension and later submission allowed, solution will be given on MyCourses before 18:30, 12.12.2021.
- A6 is a self-testing, grouping work is not suggested!
- Exam: start at 8:30, 14.12.2021

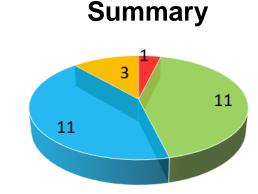


## **Assignment 05 - Summary**

Submission: 26

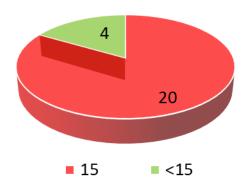
Full points: 100, is calculated as 5 points in the final grade system.

Due date: 18:00 PM, 05.12.2021 (No delayed submission)

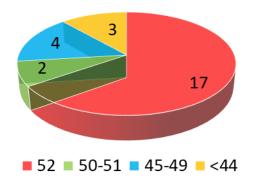


**5** 4.6-4.9 **4**-4.5 **<**4

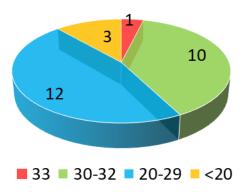
Task 1: 24, 15 points



Task 2: 26, 52 points



Task 3: 26, 33 points





### **Coordination Number and Ionic Radii**

To form a stable structure, how many anions can surround around a cation?

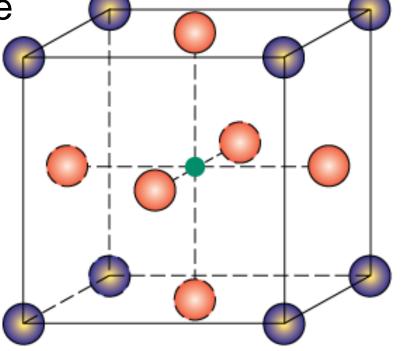
	oord. umber	ZnS (zinc blende)
< 0.155	2 linear	Adapted from Fig. 12.4, Callister & Rethwisch 10e.
0.155 - 0.225	3 triangular	NaCl (sodium
0.225 - 0.414	4 tetrahedra	chloride) Adapted from Fig. 12.2, Callister & Rethwisch 10e.
0.414 - 0.732	6 octahedra	CsCl (cesium
0.732 - 1.0  Adapted from Table  Callister & Rethwise		chloride) Adapted from Fig. 12.3, Callister & Rethwisch 10e.



## **ABX<sub>3</sub> Crystal Structures**

Perovskite structure

Ex: complex oxide BaTiO<sub>3</sub>



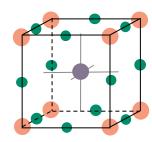


Fig. 12.6, Callister & Rethwisch 10e.

the coordination number of the  $Ba_{2+}$  ion in terms of surrounding  $Ti_{4+}$  ions is 12.





## **Case Studies**

Case Study I - Microstructure modeling

- Analyze the microstructure information of the EBSD data and create an RVE.
- Case Study II Scientific article reading and summary
- Search articles online in the focused research fields of steel, read, and write an essay to summarize the articles. Details in MyCourses Case studies
- Group work is allowed for Case Study 1. You could form a group with max. two additional peers to solve the task and provide your solution. For the convenience of grading, still submit your report individually, but indicate who your group member is. In addition, clearly state the individual contributions of each group member.
- Group work is not allowed for Case Study 2. Please finish this task independently and submit your own report.
- Common due date: 18:00 PM, 19.12.2021
- Extra 5 points for each case study in the final grading system.
- All information has been given in the task description files. As the additional case study to obtain extra points in the course, no more additional supports/resources would be given.



## Case Study 1 - Microstructure modeling

• Group work is allowed for Case Study 1. You could form a group with max. two additional peers to solve the task and provide your solution. You can submit the report in a group and clearly indicate who your group member is. In addition, clearly state the individual contributions of each group member.

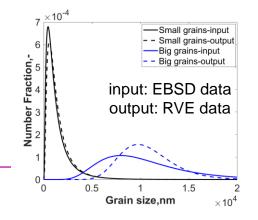
Analyze the microstructure information of the given EBSD data of a high entropy alloy (HEA) (ebsdHEA.ctf). The focused features shall be grain size and shape distribution. Use the statistical microstructure information to generate an RVE for the investigated HEA material. Analyze the microstructure information of the generated RVE (<a href="http://www.dream3d.io/Filters/ImportExportFilters/LosAlamosFFTWriter/">http://www.dream3d.io/Filters/ImportExportFilters/LosAlamosFFTWriter/</a>), assess and improve the representativeness of the generated RVE.

#### Expected results:

- The detailed analysis of the grain size and shape distribution functions and fitting.
- The procedure and results of the RVE model generation.
- An algorithm to analyze the grain size and shape distribution of the generated RVE.
- An algorithm or workflow to optimize the quality of the representativeness of the RVE model.
- Any automation algorithm of the entire process.

You might get some further information from the following papers:

W. Liu, J. Lian, N. Aravas, S. Münstermann, A strategy for synthetic microstructure generation and crystal plasticity parameter calibration of fine-grain-structured dual-phase steel, International Journal of Plasticity 126 (2020) 102614.





## Case Study 2 - Scientific article reading and summary

Table: Interesting topics/keywords in **Steel** research.

Field 1	Field 2
Microstructure	Microstructure effect on
characterization	plastic deformation
Domaga maghaniam	Fatigue property
Damage mechanism	evaluation
Strangthaning machanism	Additive Manufacturing
Strengthening mechanism	techniques
Fracture mechanics	Strain rate effect on ductile
Fracture mechanics	fracture

#### Journal list:

- Nature Reviews Materials (<a href="https://www.nature.com/natrevmats/">https://www.nature.com/natrevmats/</a>)
- PROGRESS IN MATERIALS SCIENCE
   (https://www.journals.elsevier.com/progress-in-materials-science)
- NATURE MATERIALS (<a href="https://www.nature.com/nmat/">https://www.nature.com/nmat/</a>)
- MATERIALS SCIENCE & ENGINEERING R-REPORTS
   (https://www.journals.elsevier.com/materials-science-and-engineering-r-reports)
- Annual Review of Materials Research

(<a href="https://www.annualreviews.org/loi/matsci">https://www.annualreviews.org/loi/matsci</a>)

- ADVANCED MATERIALS (<a href="https://onlinelibrary.wiley.com/journal/15214095">https://onlinelibrary.wiley.com/journal/15214095</a>)
- Materials Today (<a href="https://www.journals.elsevier.com/materials-today">https://www.journals.elsevier.com/materials-today</a>)
- ACTA MATERIALIA (<a href="https://www.journals.elsevier.com/acta-materialia">https://www.journals.elsevier.com/acta-materialia</a>)

- The review paper is acceptable.
- The selected paper shall be included in the given Journal list.
- You can also find the scientific articles from the following Journal database: <a href="https://www.sciencedirect.com/">https://www.sciencedirect.com/</a>, <a href="https://www.sciencedirect.com/"
- Case Study Deadline: 18:00 PM, 19.12.2021



## Exam - Written (70%) + Oral (30%)

Date: 14.12.2021

- 1. Join ZOOM session via desktop Client at 08:30 and turn on your microphone and video camera in order to check connections before the exam.\*
- 2. Open MyCourses MSE-Written Exam folder and **Exam question paper will be available after 08:40**. The questions are not available earlier. Read it and if needed, write question(s) in chat (the chat is used for all students' question during the exam).
- 3. Any announcements or questions will be given in ZOOM chat. You are suggested to turn off your speaker from 08:45 to 10:50 and only pay attention to the ZOOM chat.
- 4. Answer to exam questions using method most suitable to you and exam submission (e.g. handwriting, Word, Mathcad, etc.). Remember that reasoning, calculation steps, results, and discussions should be clearly visible similar to the traditional exam.
- 5. Exam starts at 08:45 and ends at 10:45. **After the exam**, you have **15 minutes** to **create a single pdf document** and deliver it using MyCourses **submission**.
- 6. The exam submission will be closed exactly at 11:00. No more extension allowed!



## Exam - Written (70%) + Oral (30%)

- 1. The oral exam will start at 11:00. All students will be divided into several groups (6-8 groups in total) by ZOOM breakout rooms, and each group has ~15 mins for questions & answers. The grouping and exact exam time for each group will be announced at 10:55-11:00 via ZOOM.
- 2. Join your breakout room and waiting for your turn for the oral exam. Your group will be cued when it is your turn through the broadcasting function. When your turn is up, leave the breakout room and come to the main room for the oral exam.
- 3. You can leave your computer physically when it is not your turn during the oral exam. But please **keep login in the ZOOM breakout rooms! Keep your microphone and video camera open** all the time even you leave your computer.
- 4. Professor will ask questions one by one. Please keep silent when the professor is talking with other students. Try to give concise answers, especially **keywords** based.
- 5. Oral exam is not an open-book exam.
- 6. Discussion is strictly prohibited during both written and oral exams.

## Exam - Written (70%) + Oral (30%)

08:30-08:45 Preparation for the exam

08:40-08:45 Exam question paper open on MyCourses

08:45-10:45 Written exam

10:45-11:00 Create one PDF file and submit.

No more extended submission after 11:00!

11:00-13:00 Oral exam (~15 mins for each group)

#### Note:

- Prepare a silent environment for your exam.
- Please login with ZOOM desktop Client (not web browser) and enable breakout rooms (<a href="https://support.zoom.us/hc/en-us/articles/206476093-Enabling-breakout-rooms">https://support.zoom.us/hc/en-us/articles/206476093-Enabling-breakout-rooms</a>).
- Keep your microphone and video camera open during the whole exam.
- Written exam is open book exam so you can utilize all materials.
- Discussion is strictly prohibited during both written and oral exams.
- Check beforehand that you have suitable tool to create single pdf file.
- Oral exam is not open-book exam.



# **Questions?**

- Assignment 6 submission DDL is 18:00 on 12.12.2021.
- Case studies submission DDL is 18:00 on 19.12.2021.
- Exam 08:30 on 14.12.2021.
- Contact: MyCourses 'General discussion' channel
- Please check the existing topics in "General discussion" before proposing a new one.
- Good luck to all of you!