Advanced Metallurgy – Case Study

Rules and guidelines

- Please **team up** with other course mates and form groups of **3-4 students.**
- Select one of the topics below for your group. Two or more groups may choose the same topic.
- The idea is to solve the problems below with the help of the Thermo-Calc software package (you may use all available modules). You are not expected to cover the topics exhaustively, but rather pick out a certain aspect and focus on that.
- The main results of the case study have to be summarized in a scientific paper in English. **Please create a suitable title for the paper that accurately reflects your chosen topic**. Please use the Word paper template provided on Moodle for the preparation of your paper, on which you can also find instructions for the paper layout.
- You will need to find and read additional literature (journal or conference papers, textbooks, reports, etc.) so that you become more familiar with the topic. The results from the literature survey have to be summarized in the Introduction part.
- For the literature search, you can use e.g. ScienceDirect, Google Scholar, Springer Link or directly search on the webpages of the most common journals (list see below). Useful information can be also found in conference proceedings or edited books, which you should be able to access via the EPFL library.
- Select your papers carefully and do not simply take the first ones that appear in your literature search. You can certainly discuss your selected papers with us.
- Write your paper in your own words and avoid copying or pasting text directly from the sources, whether in the original language or translated. **The use of AI-generated text, including ChatGPT, is strictly prohibited**. We will check for this as well as for plagiarism, and **any violations will result in a penalty**! You may use figures from the papers, but they must be properly cited.
- Length: Maximum of **10 pages**, with no more than **8 figures** (which can be sub-divided, e.g., Fig. 1a, Fig. 1b, as seen in journal papers). Extra content beyond this limit will not earn additional credit; we are primarily interested in your ability to synthesize the information from literature and your results effectively!
- The results have to be also summarized on a **Poster (A1 or A0),** which will be presented during a student seminar on the last day of lectures (18.12.2024). More information about place and time for the poster session will be provided later.
- Every group member is supposed to make a significant contribution to the paper writing and the poster presentations. There are different ways for how to do that, and it is up to you to organize yourselves. **If you encounter difficulties or have questions about distributing work packages among the group, please contact us early on.**
- We know that you are all beginners with Thermo-Calc and we do not expect the impossible from you. We will provide an "office hour" via Zoom, during which we will try to answer any technical questions you may have. The date will be announced later.

Topics case study - 2024/25

1. Alloy design
   1.1. Development High-strength Low-density Steels (Fe-Mn-Al steels)
   - Model the thermodynamics and kinetics of microalloying elements in HSLA steels.
   - Use Thermo-Calc to simulate phase stability and transformation kinetics.
   - Reason: HSLA steels are essential in construction and automotive industries. Precise modeling can enhance their performance and cost-effectiveness.

   1.2. Development of Temperature Resistant Al Superalloys
   - Use Thermo-Calc to model phase stability, precipitation behavior, and high-temperature phase equilibria in Al superalloys.
   - Explore the effects of alloying elements (e.g., Ni, Ti, V, Zr) on the mechanical properties, oxidation resistance, and thermal stability of Al superalloys.
   - Perform simulations to optimize the composition and heat treatment processes to achieve the desired balance of properties.
   - Reason: Developing temperature-resistant aluminum superalloys is crucial for advanced aerospace and automotive applications where materials are exposed to high temperatures.

   1.3. Development of Corrosion Resistant Duplex Steels
   - Investigate the specific effects of alloying elements (e.g., Mo, N, Cu) on the corrosion resistance of duplex stainless steels.
   - Utilize Thermo-Calc to predict phase equilibria and calculate pitting resistance equivalent (PRE) values for different alloy compositions.
   - Conduct simulations to determine the optimal balance of alloying elements that maximize corrosion resistance while maintaining mechanical properties.
   - Reason: Duplex stainless steels are widely used in industries requiring high corrosion resistance, such as chemical processing and marine environments.

2. Metals processing
   2.1. Microsegregation during Solidification of Duplex Stainless Steel
   - Focus on the prediction and control of microsegregation in duplex stainless steels.
   - Use Thermo-Calc to simulate solidification processes and predict phase distributions.
   - Reason: Microsegregation impacts mechanical properties and corrosion resistance.

   2.2. Casting of Steels
   - Compare the casting process of low alloyed steel, 9-12Cr steel with carbides, and high-alloyed austenitic stainless steel.
   - Perform equilibrium, Scheil, and DICTRA simulations to model solidification in various steel grades.
   - Investigate how carbides in 9-12Cr steel influence solidification compared to high-alloyed austenitic stainless steel.
   - Reason: Understanding solidification helps improve casting quality and optimize material properties.

2.3. Solidification Pathways and Segregation in Al-Si Casting - effect of impurities

- Assess the thermodynamic behavior of impurities (e.g., Fe, Si) in recycled aluminum alloys and their impact on phase stability and material properties.
- Identify strategies to mitigate the adverse effects of impurities on the mechanical properties and corrosion resistance of recycled aluminum alloys.
- Reason: Recycling is vital for sustainability in the aluminum industry. Thermodynamic assessments can improve the efficiency and quality of recycled alloys.

2.4. Dissimilar Steel Joints by Diffusion Bonding

- Investigate the diffusion bonding behavior of tool steel (1.2363/X100CrMoV5) with low alloy steels (C<0.08%) at temperatures above 1000°C.
- Analyze the effects of temperature and time on the material interface during the bonding process.
- Study the changes in microstructure and phase distribution at the interface between the two steel types.
- Explore how elements like carbon, chromium, molybdenum, and vanadium influence the diffusion and bonding quality.
- Consider the implications of the diffusion process on mechanical properties such as hardness and strength of the bonded materials.
- Reason: Understanding the interface behavior is crucial for optimizing bonding processes in applications requiring strong metallurgical joints.

3. Heat treatments

3.1. Kinetics of Phase Transformations in Fe-Cr-Ni Alloys

- Investigate the kinetics of austenite to martensite transformation in Fe-Cr-Ni alloys.
- Employ DICTRA for diffusion-controlled phase transformations.
- Reason: Understanding phase transformation kinetics is vital for tailoring mechanical properties.

3.2. Precipitation Hardening in Al-Mg-Si Alloys

- Study the precipitation sequence and kinetics in Al-Mg-Si alloys.
- Use TC-PRISMA module in Thermo-Calc for nucleation, growth, and coarsening simulations.
- Reason: Precipitation hardening significantly enhances the strength of aluminum alloys.

3.3. Nucleation and Growth of Intermetallic Phases in Al-Cu Alloys

- Explore the formation and growth of intermetallic phases in Al-Cu alloys.
- Use TC-PRISMA and DICTRA for concurrent nucleation and growth simulations.
- Reason: Intermetallic phases can significantly influence the mechanical properties of Al-Cu alloys.

3.4. Impact of Ageing Treatmet on the Yield Strength and Hardness of Al-Mg-(Sc,Zr) alloys

- Literature review on precipitate formation the commercial heat treatments of Al-Mg-(Sc,Zr) alloys and simulation of the aforementioned heat treatments
- Comparison of the obtained hardness and yield strength values

- Comparison of the impact of the different hardnening mechanisms (precipitation hardnening, solid solution strengthening and grain boundary strengthening) for the different available heat treatments
- Reason: Understanding how ageing treatments influence mechanical properties is essential for optimizing the performance of Al-Mg-(Sc,Zr) alloys.

3.5. Heat Treatment of Fe-Mn-C steel

- Investigate carbide formation in medium and high Mn steels as a function of time and temperature.
- Analyze the impact of small additions of elements like Nb, V, and Ti (<1 wt.%) on carbide formation.
- Reason: Understanding carbide formation and the role of alloying elements is crucial for optimizing the heat treatment of Fe-Mn-C steels.

4. Alloy performance in service

4.1. High-Temperature Oxidation Behavior of Fe-Ni-Cr Alloys

- Investigate the high-temperature oxidation mechanisms and kinetics of Fe-Ni-Cr alloys.
- Utilize the metal slag and oxide database in Thermo-Calc to predict the formation and growth of oxides such as $Cr2O3$, $Fe2O3$, and NiO.
- Study the impact of different alloying elements (e.g., Al, Si, Ti) on the oxidation resistance.
- Reason: Fe-Ni-Cr alloys are widely used in power generation and aerospace due to their excellent high-temperature mechanical properties and oxidation resistance.

4.2. Sensitization of Steels

- Define sensitization of stainless steels and identify its causes.
- Explain how a) heat treatment or b) modifying the composition of X10CrNi 18-8 steel can reduce the risk of sensitization, and the reasons behind these methods.
- Reason: Understanding and preventing sensitization is crucial for maintaining the corrosion resistance and long-term performance of stainless steels in various applications.

4.3. Diffusion Processes in Cu-based Alloys for Electronic Applications

- Analyze diffusion processes in Cu-based alloys, focusing on applications in electronics.
- Use Thermo-Calc to simulate interdiffusion and homogenization kinetics.
- Reason: Control over diffusion processes can enhance performance and reliability of Cu-based electronic interconnects.

5. Primary and secondary metallurgy

5.1. Deoxidation and Inclusion Control in stainless steels

- Study the deoxidation practices and inclusion control during the primary and secondary metallurgy of stainless steels.
- Use Thermo-Calc to simulate the thermodynamics of deoxidation reactions and predict the formation of various inclusions (e.g., oxides, sulfides).
- Evaluate the impact of different deoxidizers (e.g., Al, Si, Mn) and their combinations on the cleanliness and mechanical properties of stainless steels.

- Reason: Understanding the thermodynamics and kinetics of deoxidation and inclusion formation can help optimize steelmaking practices, resulting in cleaner steels with improved strength and toughness.

5.2. Impact of impurity elements on the recycling-secondary metallurgy of (stainless) steel

- Conduct a literature survey on the main impurities in recycled stainless steel, their origins, and their impact on mechanical and thermophysical properties.
- Use Thermo-Calc to simulate the solidification microstructure of stainless steel containing impurities.
- Propose heat treatments using Thermo-Calc to modify the microstructure post-casting, aiming to match the microstructure of 316L without impurities.
- Reason: Understanding the effect of impurities is essential for improving the quality of recycled stainless steel through optimized secondary metallurgy processes.

Journals in the field of metallurgy (the list is not exhaustive)

- Acta Materialia
- Scripta Materialia
- Materials and Design
- Materials Science and Engineering A
- Materials Characterization
- Intermetallics
- Journal of Materials Research and Technology
- Journal of Alloys and Compounds
- Journal of Materials Research and Technology
- Materials and Metallurgical Transactions A
- Journal of Materials Processing Technology
- Advanced Engineering Materials
- MDPI Metals
- MDPI Materials
- …

Contact information

- Please inform us by e-mail to Jian Yang (jian.yang@epfl.ch) and Seyyed Ezzatollah Moosavi (ezzatollah.moosavi@epfl.ch) until **25.09.2024 latest** with whom you want to team up and which topic you want to choose.
- You can certainly contact us if you have questions regarding the literature search or the topic.