

1 390 Problems

1.1 Materials Selection in Mechanical Design

Note: Because the CES Materials Selector Software only works on PCs, which not everyone has, these projects will be done in your project groups, with 1 report submitted per group. Upload the completed report to Canvas as a pdf file on the due date.

In order to receive credit for the CES materials selection problems, you must:

- answer the questions
- explain the process used to get your answers
- include ALL relevant CES plots with explanations of the information given on each plot in all problems. CES plots should be properly enlarged in specific regions if needed, and failed records of materials (materials that do not satisfy the criteria shown in gray) should be hidden.

There is no unique answer to the questions. Therefore, your grade will not be determined by the particular materials you choose. You can select any materials that satisfy the criteria and as long as you explain the process used to get your answer.

Start from “Level 3” database and “All bulk materials” for all problems.

To change units go to: tools → settings → units → <automatic-metric> or <metric>

1) General use of the CES database: Answer the following using CES database:

- (a) A component is currently made of soft commercially pure Gold. Due to high cost of gold, please use CES to suggest two other materials that have greater thermal conductivity.
- (b) Find a material with $250 < E < 350$ GPa and density $7,000 < \rho < 8,000$ kg/m³.
- (c) Which have higher specific stiffness, E/ρ : titanium alloys or tungsten carbides?
(Hint: use 'Tree' in the selection stage to select titanium alloys and tungsten carbides only)
- (d) Is the fracture toughness, K_{IC} , of common engineering polymers like PVC elastomer (Shore A60) higher or lower than those of engineering ceramics like silicon carbide (HIP)?

2) Multi-stage materials selection using CES database You are employed by a company that manufactures various sports goods except tennis rackets. Even though the company is doing well, in an effort to expand company's market the management decided to introduce a new product: tennis rackets. Being the only Materials Engineer in the company your new assignment is to select four different materials that would be suitable for manufacturing tennis rackets.

Since you have already used CES, you should not have any problem in getting started. First, let us examine the essential functions of a body of a tennis racket: structural support for the string, transfer of force, absorption of energy (damping) etc. Often, the tennis rackets are also subjected to mechanical abuse (due to bad temper or frustration of the players). Thus, the optimal materials must be light, stiff, strong, and should have reasonably good fracture toughness. In conjunction with the CES database, the following multi-stage criteria may be applied to select off-the-shelf materials suitable for manufacturing tennis rackets.

Stage I: Assume that due to the complex shape of the body of the tennis racket the maximum stiffness at minimum weight is given by the following performance index:

$$M_1 = \frac{\sqrt{E}}{\rho} \quad (1.1)$$

where E is the Young's Modulus, and ρ is the density.

Stage II: The maximum ductile strength of rods at minimum weight is given by the following performance index:

$$M_2 = \frac{\sigma_y^{0.8}}{\rho} \quad (1.2)$$

where σ_y is the yield stress (Elastic Limit in CES).

Stage III: The maximum fracture toughness of rods at minimum weight is given by the following performance index:

$$M_3 = \frac{K_{IC}}{\rho} \quad (1.3)$$

where K_{IC} is the fracture toughness.

Stage IV: Selection of materials that will give minimum density and maximum damping capacity. In CES, the damping behavior is represented by the Mechanical Loss Coefficient under Optical, aesthetic and acoustic properties. A higher mechanical loss coefficient implies a better damping capacity. Use Box Method for selecting a subset of materials (with $\rho < 2,000 \text{ kg/m}^3$ and mechanical loss coefficient greater than 0.008) in this stage.

Use the above four stages of selection to determine the optimal materials for tennis racquets. The materials must also satisfy the following:

- $M_1 > (10^3 \text{ Pa})^{0.5}/(\text{kg}/\text{m}^3)$
- $M_2 > (10^4 \text{ Pa})^{0.8}/(\text{kg}/\text{m}^3)$
- $M_3 > (10^4 \text{ Pa}\sqrt{\text{m}})/(\text{kg}/\text{m}^3)$

(See the note in section ?? to better understand how to interpret these values of the performance index).

Turn in the following:

- Graphical output for each stage showing the selection line/box. In the report, you must explain how you have drawn the selection line in each stage;
- Table for Materials passing 4 of the 4 stages
- Select four different materials that passed all the stages for manufacturing tennis rackets. At this stage you may consider cost (listed in CES) so that rackets will have a wide range of price. List the Young's modulus, the yield stress, the fracture toughness, the loss coefficient, and price of the materials you selected, in a table like the one outlined below:

Material	E (Pa)	σ_y (Pa)	K_{IC} ($\text{MPa}\sqrt{\text{m}}$)	Mech. Loss Coeff.	Price

3) Multi-stage materials selection using CES database: As an engineer at a minor aircraft company, you have been given the task of determining the proper material for use as an aircraft door. After research you have determined nine properties that the material must possess. They are as follow:

- Fracture toughness, $K_{IC} > 40 \text{ MPa}\sqrt{\text{m}}$
- Young's Modulus, $E > 100 \text{ GPa}$
- Density, $\rho < 5,000 \text{ kg}/\text{m}^3$
- Thermal Expansion $< 20 \times 10^{-6}/^\circ\text{C}$
- Elongation $> 10 \%$
- Cost $< 20 \text{ USD}/\text{kg}$

- Recycle fraction in current supply $> 20\%$
- Flammability = {non-flammable}
- Durability in fresh water = {excellent}

Determine a suitable material for this application

1.2 Thermo-Calc

Requirements for Thermo-Calc questions:

- Your answers to all of questions must be substantiated by calculated diagrams and I should be able to make out as to what you have to plot in the figure(s)
- Everyone must submit his/her own calculated diagram(s)
- The title of the phase diagrams MUST be your name
- All phase fields must be labeled; and (v) a copy of the equilibrium results obtained from the TC 2017b window must accompany the answers that require equilibrium calculations
- You will receive an automatic zero if it is found that you have submitted someone else's phase diagram or graph.
- **Warning:** The phase labeling function of TC2017b occasionally gives you obviously wrong results. You may try removing all labels and adding them again, or adjusting window/graph sizes. If you can't get it right from the software, clarify the situation and give your answers in your homework.

4) Pb-Sn solders are widely used in electronic packaging (chip-to-chip and chip-to-carrier interconnections) and various other applications related to soldering. However, due to toxicity of Pb and environmental concerns, Pb-Sn solders have been banned in many applications, such as, food packaging (e.g., beverage cans), certain plumbing applications etc. The Sn-In phase diagram is important for designing multicomponent Pb-free solders.

Hints: (i) Use SSOL2 database; (ii) For both the Pb-Sn and In-Sn systems, consider the following phases only: LIQUID, FCC_A1 and BCT_A5; (iii) temperature limits for mapping: $0 - 400^\circ\text{C}$ for both alloys. In the SSOL database, the Sn-phase is defined by BCT_A5, because its structure is body centered tetragonal, the In-phase and Pb-phase are defined by FCC_A1, because both of their structures are face centered cubic.

- (a) Calculate Pb-Sn and In-Sn equilibrium phase diagrams. You have to submit the calculated phase diagrams with all phase fields labeled.
- (b) What are the calculated eutectic temperatures in Pb-Sn and In-Sn systems?
- (c) What are the calculated solid solubilities of Pb in Sn and In in Sn at their respective eutectic temperatures? Answer this question both in weight and atomic percents of Pb and In.
- (d) Despite toxicity/environmental concerns, Pb-Sn solders are widely used in all microelectronic packages. In particular, the Pb-Sn eutectic alloy. For a Sn-38 wt.% Pb alloy, answer the following:
- i What are the phases present at 50 ° C and 130 ° C? (Note: many devices, such as computers operate in this temperature range)
 - ii What are the amounts and composition (in wt%) of the phases present at 50 and 130 ° C?
 - iii What are the important differences you notice between the calculated results at these two temperatures?

5) Calculation of the Ms temperature (temperature when martensite starts to form) is a very crucial step in designing ultra-high strength, secondary hardening martensitic steels. Such a calculation allows us to select the alloy(s) whose Ms is sufficiently high so that upon quenching (from solution treatment temperature) to room temperature a fully martensitic microstructure is obtained. If the Ms is not high enough, then we may get incomplete transformation at room temperature and the alloy will need to be quenched at sub-ambient temperatures. Therefore, an alloy with an $M_s > 300^\circ\text{C}$ would be desirable.

Hints: (i) Use the SSOL2 database; (ii) consider the following phases for 2.1-2.4: BCC_A2 and FCC_A1, consider the following phases for 2.5: LIQUID, BCC_A2, FCC_A1, HCP_A3, SIGMA, CEMENTITE, M23C6, and M7C3 (iii) stepping ranges for 2.1-2.4: 200 to 1000°C for temperature; mapping ranges for 2.5: 750 to 1250°C for temperature (iv) A solution treatment temperature is defined as the temperature at which all solutes will be in solid solution in one phase.

The alloy is based on iron with different concentrations of C, and with 14 wt. % Co, 8 wt. % Cr, 6 wt% Ni, 0.5 wt. % Mo and 0.3 wt. % V.

- (a) What is the T_0 temperature of the above alloy as a function of C content? Consider carbon concentrations 0.1 wt%, 0.3 wt%, 0.5 wt%, 0.7wt% and 0.9 wt%?
- (b) Comment of the effect of C on the T_0 temperature.
- (c) Assuming that the martensitic transformation starts at a Driving Force of -1500 J/mol, what is the M_s temperature of the above alloy as a function of C content at 0.1 wt%, 0.3 wt%, 0.5 wt%, 0.7wt% and 0.9 wt%?
- (d) Comment on the compositional dependence of M_s temperatures and determine which alloy(s) would be appropriate for the application stated in the above question.
- (e) Calculate the vertical section of this alloy. For a solution treatment temperature of 1000°C, what is the maximum amount of C that can be put in the alloy? Show this point of the phase diagram.

1.3 DICTRA

To receive credit:

- Your answers to all of questions must be substantiated by calculated diagrams or table renderer results
 - everyone must submit his/her own calculated diagram(s)
 - the title of the phase diagrams MUST be your name
- 6)** γ to α transformation in a ternary Fe-0.15wt%C-0.50wt%Si steel, when cooled from 1173K down to 1050K with the cooling rate of 10K/minute, and then isothermally held at 1050K until total heat-treatment time reaches 107 sec.
- (a) Provide a plot of carbon concentration vs distance at $t=1000$, 100000, 107 sec.
- (b) Provide a plot of silicon concentration vs distance at $t=1000$, 100000, 107 sec. Compare with the plot of the carbon concentration. Which element do you think is more mobile in this steel at this temperature, C or Si?

Hints:

- Use the SSOL2 database as thermodynamics database, and MOB1 database as mobility database
- Consider the following phases: FCC_A1 (γ , austenite) and BCC_A2 (α , ferrite)
- assume fully homogenized austenite (FCC_A1) at the beginning of the heat-treatment
- apply 50 grid-points of geometric grid with ratio = 1.05 in the initial austenite region
- assume ferrite starts to form when the driving force exceeds 10⁻⁵ (vi) use potential (not activity) for finding tie-line at the phase interface

1.4 TC-PRISMA**To receive credit:**

- Your answers to all of questions must be substantiated by calculated diagrams or table renderer results
- everyone must submit his/her own calculated diagram(s)
- the title of the phase diagrams MUST be your name

1.4.1

Isothermal precipitation calculation of γ - γ' Ni-12Al (at%) alloy at 450 °C for 1e15 s

Hints:

- Use the Demo Ni alloys database package
 - Consider the following phases: DIS_FCC_A1 (matrix) and FCC_L12#2 (precipitate)
 - Precipitate nucleation sites: bulk, interfacial energy 0.035 J/m²
- (a) What is the maximum number density of precipitate? How long does it take to reach the maximum number density of precipitates (in hours)?
- (b) What is the volume fraction of precipitate phase and matrix composition (Al concentration in at%) at 1e15 s?

1.4.2

3. Isothermal precipitation calculation of metastable and stable carbides in Fe-0.1C-12Cr (wt%) at 750 °C for 1e6 s

- (a) From the volume fraction vs. time figure, can you tell the sequence of precipitation?

Hints:

- Use the Steel and Fe alloys database package;
 - consider the following phases: BCC_A2 (matrix), CEMENTITE (precipitate), M23C6 (precipitate), and M7C3 (precipitate)
 - precipitate nucleation sites: grain boundaries
 - interfacial energy: CEMENTITE (0.167 J/m²), M23C6 (0.252 J/m²), M7C3 (0.282 J/m²)
 - plot volume fraction of all three carbides (linear) vs. time (log 10)
- (b) Can you obtain this precipitation sequence without doing this isothermal calculation?

Hint:

Example 2 in Lab 5b tutorial

- (c) What the volume fraction of the stable precipitate phase at 1e6 s? How about its equilibrium volume fraction?

Hint:

TC single point equilibrium calculation using TCFE9 database with BCC_A2, CEMENTITE, M23C6, and M7C3 entered