

3.020, Spring 2021

Thermodynamics of Materials

Problem Set 3

Massachusetts Institute of Technology
Department of Materials Science and Engineering

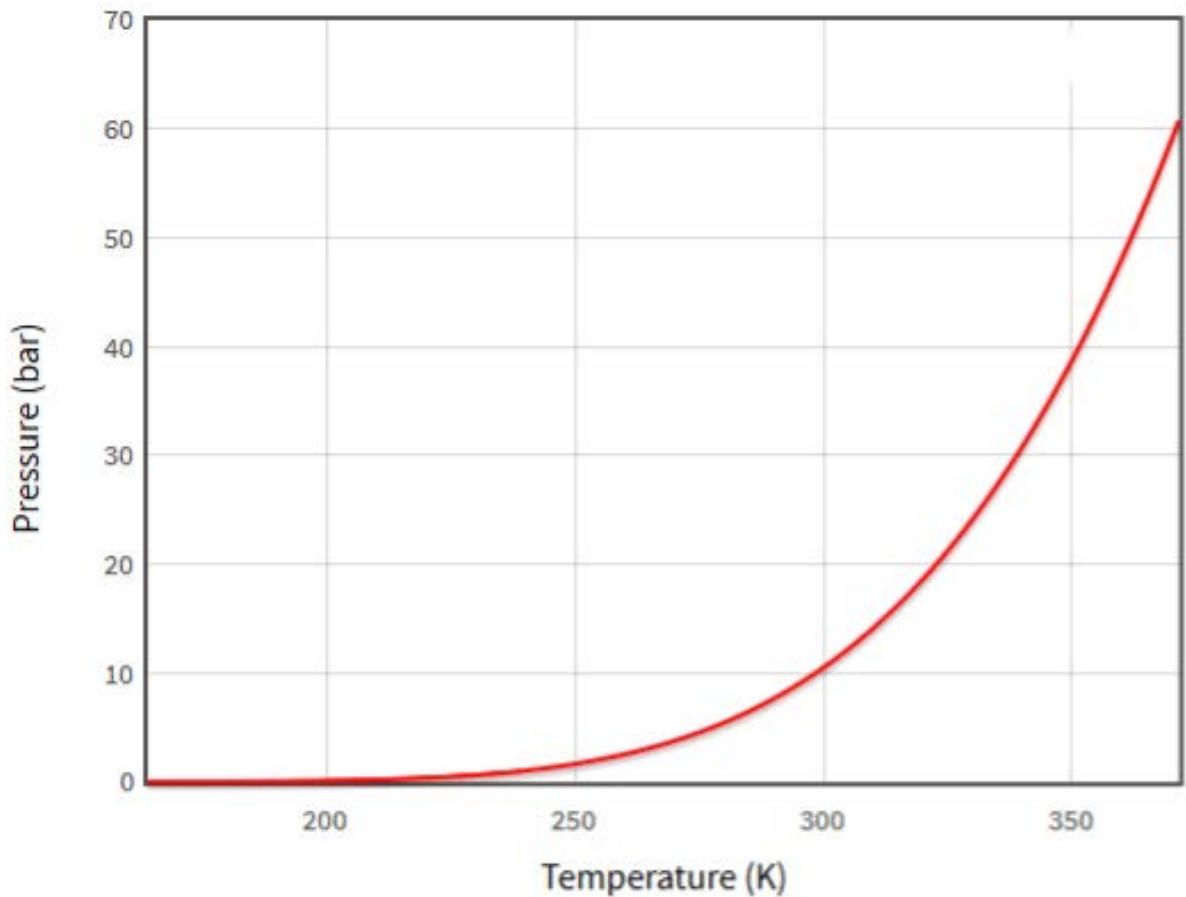
Due March 19, 2021 at 10am EST

We encourage you to work in groups. If you do so, please note the names of your groupmates on the first page of your solutions.

Remember to clearly present your solutions, including intermediate steps. We have provided a lot of space for each problem in this document, so please make use of it. Failure to show your work may result in reduced credit. Sloppy presentation may result in reduced credit.

3.1: Fun with the C-C equation [7 pts]

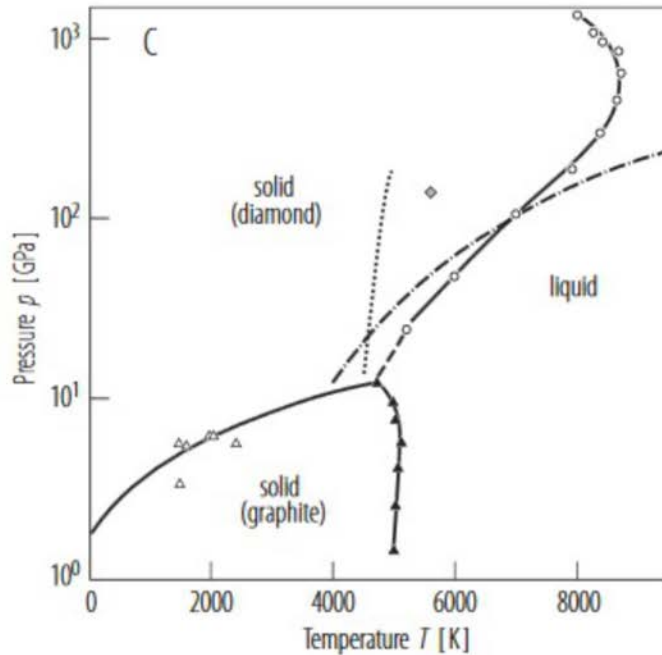
Here is a plot of the saturation vapor pressure of a fairly common substance:



- (a) Can you tell from this plot alone if this corresponds to an evaporation or sublimation transformation? [0.5 pt]
- (b) What pressure is needed to fully condense this substance at 300 K? [1 pt]
- (c) Estimate the enthalpy change of evaporation/sublimation. [5 pt]
- (d) What is this substance ? [0.5 pt]

3.2: Heating and squeezing solid phases [12 pts]

Here is the phase diagram of carbon:



Landolt-Börnstein - Group III Condensed Matter
 44D (New Data and Updates for IV-IV, III-V, II-
 VI and I-VII Compounds, their Mixed Crystals and
 Diluted Magnetic Semiconductors)
 10.1007/978-3-642-14148-5_160 (Springer-Verlag
 Berlin Heidelberg © 2011)

- Sketch a plausible plot of the enthalpy as a function of T in the range of 0-8000 K at fixed $P = 3$ GPa. You should indicate values on the abscissa (the T axis), but your ordinate (the H axis) does not need tick marks or specified values. You don't need the numerical values of $H(T)$, but your plot should be consistent with thermodynamic principles. [2 pts]
- Sketch a plausible plot of the entropy as a function of P in the range 1-100 GPa at fixed $T = 2000$ K. As before, you should indicate values on the abscissa, but your ordinate does not need tick marks or specified values. You don't need the numerical values of $S(P)$, but your plot should be consistent with thermodynamic principles. [2 pts]
- Using real thermodynamic data, calculate the change in Gibbs free energy for isothermal compression of 1 mole of graphite from 1 to 10 bar at 25°C . As always, for full credit indicate the source of your data, maintain best-practices with significant figures, and clearly state your assumptions. [4 pts]
- Now consider isobaric cooling of 1 mole of graphite at 1 bar, starting at 25°C . What temperature change is needed to produce the same change in G that you calculated in part (c)? [4 pts]

3.3: The mystery phase diagram problem [11 pts]

You are heading a team studying two phases of exciting new material Entropium, names Lunite and Solite. One of your researchers pulled an all-nighter working on the materials and is a little fuzzy on some of the details from his work. He is confident of the following information:

- When heating the Entropium at any constant pressure, 10 kJ/mol of heat was either required or released (he can't remember which) to completely convert the Entropium from one of the two phases to the other once he had reached the temperature of the transition.
- At 300 bar and 645°C as well as 100 bar and 520°C , Lunite and Solite can coexist in equilibrium. 1 bar = 100 kPa.

- (c) He was capable of producing both Lunite and Solite from a previously characterized metastable phase of Entropium known as Duskite at a temperature and pressure that he cannot remember. He knows it required heat to convert Duskite into Lunite, but heat was released by the conversion of Duskite to Solite.
- (d) The two phases have the same coefficient of thermal expansion, compressibility, and heat capacity.
- (e) The highest melting point of either Lunite or Solite at 1 atm is 1400 °C. Enthalpy of fusion for this phase is 25 kJ/mol.

After sending the researcher home to get some sleep, and scheduling a team-wide meeting on how to keep a proper lab notebook, you attempt to determine what you can about Lunite and Solite. Please do not make additional assumptions.

- (a) What is $\Delta H^{\text{Lunite} \rightarrow \text{Solite}}$? [2 pts]
- (b) Based on your answer in part a, which of the two phases must be stable at lower temperatures? [2 pts]
- (c) What is $\Delta V^{\text{Lunite} \rightarrow \text{Solite}}$? [2 pts]
- (d) What is the equilibrium phase transition temperature between Lunite and Solite at atmospheric pressure? [2 pts]
- (e) If the lower temperature of the two phases could be superheated past conversion to the higher temperature phase, at what temperature would you expect the lower temperature phase to melt at 1 atm? [3 pts]

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