

Engineering 45
The Structure and Properties of Materials
Midterm Exam Solutions
March 22, 2006

Problem 1: (35 points)

(a) (5 points) Describe the β -ZnS structure and show how it is related to the FCC structure.

See Fig 3.40 on page 64 of Morris notes.

(b) (10 points) The β -ZnS structure is adopted by many covalently bonded compounds, like GaAs. Why would this structure be favored? [Ga has valence 3, As has valence 5.]

GaAs has an average valence of 4 electrons. The β -ZnS structure is such that all atoms have four nearest neighbors arranged in a tetragonal structure. Thus, in this structure GaAs can saturate all of its bonds by sharing one atom per bond with each of its nearest neighbors, which is the definition of covalent bonding.

(c) (10 points) The β -ZnS structure is also adopted by some ionic compounds, like AgI. What characteristic of these compounds would favor V over other ionic structures?

Since all of the neighbors of an FCC atom in the beta-ZnS structure are tetrahedral atoms, and vice versa, the structure is a natural fit for equi-valent ionic compounds. This maintains charge neutrality in the unit cell and minimizes like-ion repulsion. Specifically, the preference for beta-ZnS over other ionic structures like NaCl or CsCl is due to the size ratio of the ions.

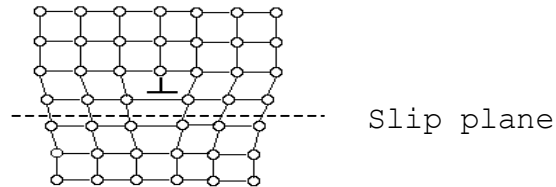
(d) (10 points) Under what conditions might a metallic AB compound choose the β -ZnS structure?

A metallic AB compound might choose the beta-ZnS structure if there is a significant size difference between the A and B atoms such that this structure provides the most ideal close-packing. This would occur if the ratio of $R(\text{tetrahedral})$ to $R(\text{FCC})$ atoms lies between about 0.225 and 0.414. In addition, a metallic compound would have to prefer an ordered structure rather than random solid solution of A & B atoms; usually this occurs at lower temperatures where entropy does not dominate the overall free energy of the crystal.

Problem 2: (30 points)

(a) (5 points) Draw and edge dislocation in a simple cubic crystal.

An edge dislocation in a simple cubic structure



(b) (5 points) Show how the glide of that dislocation produces plastic deformation.

See Figures 4.7 and 4.8 in Morris Notes.

(c) (10 points) Define the “climb” of an edge dislocation and explain why it is difficult for an edge dislocation to climb unless the temperature is high.

Climb of an edge dislocation is the movement of the dislocation in a direction out of the glide plane. Depending on the direction (“up” or “down”) atoms are either liberated or adsorbed from the extra half-plane of atoms that defines the dislocation line. This process is difficult unless at high temperatures because the absorbing vacancies from the lattice and the diffusion of atoms into these vacancies is required. The equilibrium concentration of vacancies is higher at higher temperatures. The diffusion of atoms/vacancies is also relatively easy at higher temperatures due to thermal activation.

(d) (10 points) When a metal is severely deformed the diffusivity of substitutional species within it usually increases significantly, and remains high for some period of time after the deformation is finished. Why?

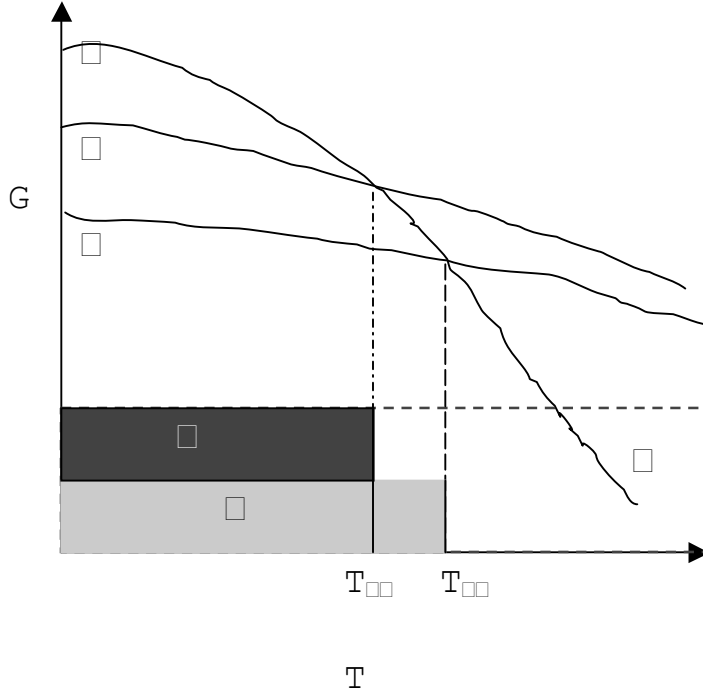
Severe deformation of a metal results in the increase of vacancies in the lattice. The diffusion of substitutional species requires the presence of vacancies since it can only jump to a neighboring site if the site is vacant. This is why there is a significant increase in the diffusivity of substitutional species for some period of time after the metal was severely deformed. The diffusion rate for the substitutional species will remain high until the species preferentially migrate to defects in the lattice such as dislocations and grain boundaries to relieve strain.

Note: The problem did not ask about interstitial species or effects of temperature.

Problem 3: (35 points)

A one-component material has three possible structures, α , β , and γ . At high T the system is α . If it is cooled slowly it transforms to β at $T < T_{\alpha\beta}$, and remains β for all lower temperatures. If it is cooled quickly it transforms to γ at $T_{\alpha\gamma} < T_{\alpha\beta}$.

(a) (5 points) Suppose that both the $\alpha \rightarrow \beta$ and $\alpha \rightarrow \gamma$ transformations occur by nucleation and growth. Sketch plausible forms of the free energy vs. temperature curves for the three phases that might lead to this behavior.



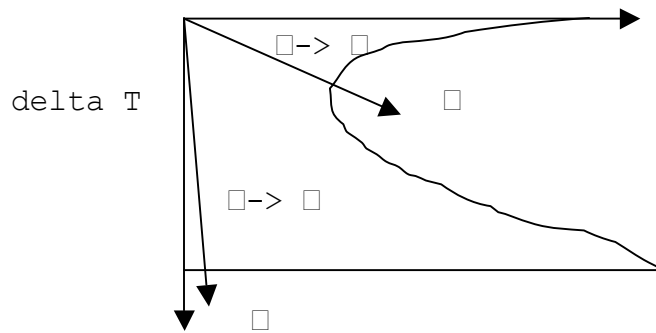
(b) (10 points) Are the kinetics of this transformation more likely governed by fig. (a) or fig. (b)? Explain.

There was some ambiguity in this question and as such two possible solutions are correct if accompanied by a proper explanation that supports your choice.

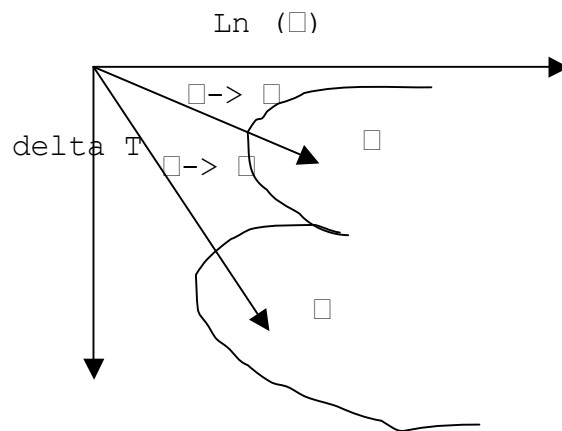
If you assume the conditions as stated in the original question, “If it is cooled slowly it transforms to β at $T < T_{\alpha\beta}$, and remains β for all lower temperatures. If it is cooled quickly it transforms to γ at $T_{\alpha\gamma} < T_{\alpha\beta}$,” then the kinetics of the transformation are governed by fig. (b).

If the material is cooled slowly, there is enough time for the nucleation of β from the α phase and the growth of the new β precipitates. Since the kinetics are governed by nucleation and growth, there should be a “C-shaped” curve in the TTT diagram. If the material is cooled quickly, there is

not enough time for nucleation and growth to happen so the transformation will be suppressed and miss the nose of the “C-shaped” curve and reach γ phase directly. As shown in 3a), γ phase is metastable, so transformation of the γ phase is not governed by nucleation and growth, therefore the γ phase region in a TTT diagram will be a straight horizontal line. Figure (b) shows a “C-shaped” curve and one horizontal line so the answer should be Figure (b).



If you assumed the conditions as stated in 3(a), “Both the $\alpha \rightarrow \beta$ and $\alpha \rightarrow \gamma$ transformations occur by nucleation and growth”, the kinetics of the transformation are more likely governed by fig. (a). Since the transformations occur by nucleation and growth, it needs time for either nuclei of β or γ to nucleate out of the α phase and the new β phase (or γ phase) can diffuse to make the nuclei grow. Therefore there should be two “C-shaped” curves in the TTT diagram.



(c) (10 points) Now assume that phase α is a liquid, phase β is a crystalline solid and phase γ is a glass. Are the kinetics of the transformation more likely governed by (a) or (b) in this case? Explain.

The kinetics of this phase transformation are governed by Figure b. Figure b indicates that the transformation from alpha to beta is governed by nucleation and growth as indicated by the “C”

shaped curve, while the transformation from alpha to gamma is indicated as a horizontal line. This horizontal line indicates that the alpha to gamma transformation is a diffusionless transformation. This is appropriate for glass (gamma) formation because a glass is formed when you cool a material so rapidly that crystallization cannot occur because diffusion is limited. Thus, glass formation is a time independent process and is represented by an isothermal line. To form the glass you have to effectively "freeze" the atoms where they are.

(d) (10 points) *While it is possible to suppress the $\alpha \rightarrow \beta$ transformation by rapid cooling, it is not ordinarily possible to suppress the $\beta \rightarrow \alpha$ transformation by rapid heating. Why?*

It is not possible to suppress the beta \rightarrow alpha transformation on rapid heating because as the temperature increases, the thermodynamic driving force for the transformation increases and the ability of the atoms to diffuse through the material also increases.

3pts were given for copying an explanation directly from the Morris notes. To receive full credit, students had to include the thermodynamic driving force and diffusion in their explanations.