

# Metallic Materials

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## 1

### 1.1

**A Pb–60 at% Sn alloy was slowly cooled from 380°C to 50°C. Calculate the volume fraction of the primary phase at 50°C.**

The phase diagram for an alloy of Pb and Sn is shown in figure 1. The temperature and composition are located in the diagram, the composition  $C_0$  corresponds to a 60% of Sn and 40% of Pb. From the figure, it can be seen that for a temperature of 50°C there is presence of two phases,  $\alpha$  and  $\beta$ . From the isothermal of the temperature it is possible to obtain the values of the compositions for each phase by intersecting the isothermal line with the boundaries of the phase diagram, which gives the following results:

$$\begin{aligned}C_{Sn_\alpha} &= 4\% \\C_{Sn_\beta} &= 99\% \\C_{Pb_\alpha} &= 96\% \\C_{Pb_\beta} &= 1\%,\end{aligned}\tag{1}$$

where  $C_{Sn_\alpha}$  is the composition of Sn in the  $\alpha$  phase,  $C_{Sn_\beta}$  is the composition of Sn in the  $\beta$  phase,  $C_{Pb_\alpha}$  the composition of Pb in the  $\alpha$  phase and,  $C_{Pb_\beta}$  is the composition of Pb in the  $\beta$  phase.

The primary phase is the phase that has a higher fraction in the mixture, for which is necessary to calculate the fraction of each phase, and to do that the lever rule is used. The lever rule states that the phase fraction can be calculated taking the distance of the tie line of the total composition to the border of the other phase and divide this by the total distance of the tie line, the expressions for the mass fractions are presented in the following equations:

$$W_\alpha = \frac{C_\beta - C_0}{C_\beta - C_\alpha}\tag{2}$$

and

$$W_\beta = \frac{C_0 - C_\alpha}{C_\beta - C_\alpha}; \quad (3)$$

where  $W_\alpha$  is the fraction of the  $\alpha$  phase,  $W_\beta$  is the fraction of the  $\beta$  phase,  $C_\alpha$  and  $C_\beta$  are the compositions of the  $\alpha$  and  $\beta$  phases, and  $C_0$  is the initial composition (Callister & Rethwisch, 2010, p. 290-291).

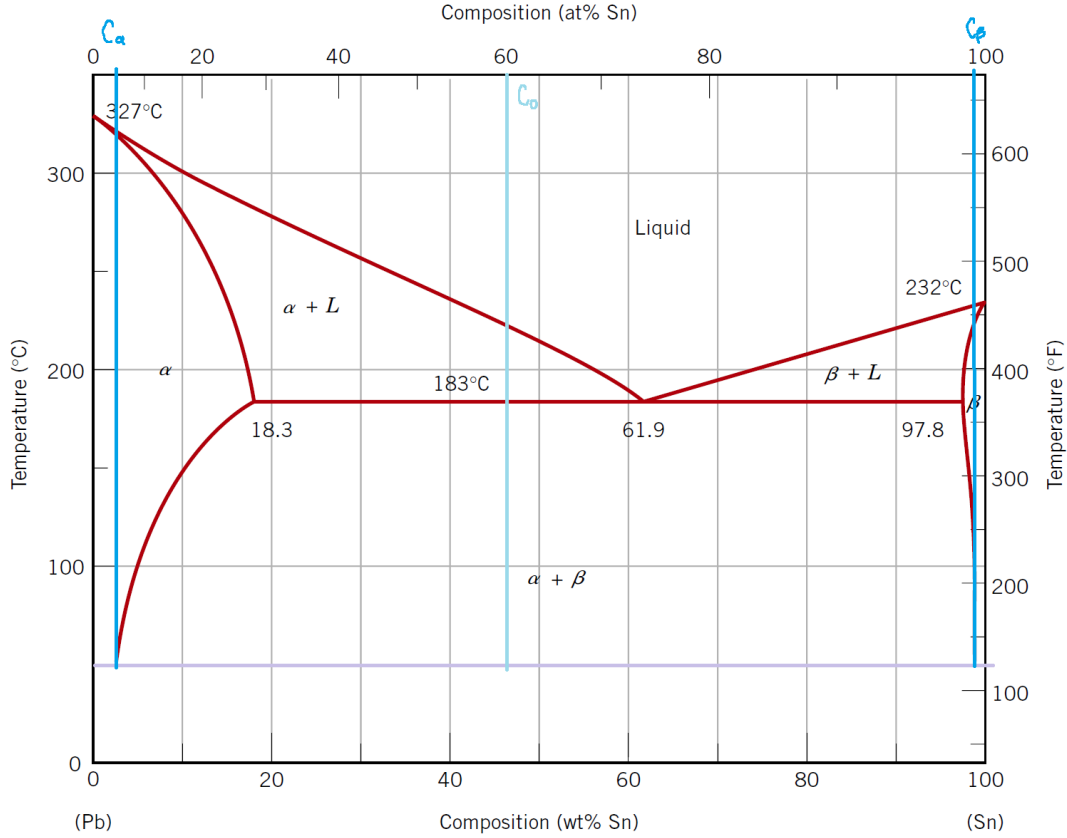


Figure 1: Phase diagram for lead-tin with the initial composition  $C_0$ , and phase compositions  $C_\alpha$  and  $C_\beta$ .

Source: Figure adapted from Callister and Rethwisch (2010, p. 300)

Using the values of the compositions for Sn from equation 1 obtained from the phase diagram in figure 1, the fractions for  $\alpha$  and  $\beta$  phases are calculated using equations (2) and (3):

$$W_\alpha = \frac{C_\beta - C_0}{C_\beta - C_\alpha} = \frac{99 - 60}{99 - 4} = \frac{39}{95} = 0.410526 \quad (4)$$

$$W_\beta = \frac{C_0 - C_\alpha}{C_\beta - C_\alpha} = \frac{60 - 4}{99 - 4} = \frac{56}{95} = 0.589474 \quad (5)$$

Based on the results obtained, it can be determined that the primary phase, the one that has a higher fraction, is the  $\beta$  phase. The equation for the volumen fraction for the  $\beta$  phase is given by:

$$V_{\beta} = \frac{\frac{W_{\beta}}{\rho_{\beta}}}{\frac{W_{\alpha}}{\rho_{\alpha}} + \frac{W_{\beta}}{\rho_{\beta}}}, \quad (6)$$

where  $V_{\beta}$  is the volumen fraction of the  $\beta$  phase,  $W_{\alpha}$  and  $W_{\beta}$  are the fractions of both  $\alpha$  and  $\beta$  phases, and  $\rho_{\alpha}$  and  $\rho_{\beta}$  are the densities of  $\alpha$  and  $\beta$  phases respectively (Callister & Rethwisch, 2010, p. 293).

From equation (6) it can be seen that it is necessary to calculate the density of each phase, which can be done by using the following equations:

$$\rho_{\alpha} = \frac{100}{\frac{C_{Sn_{\alpha}}}{\rho_{Sn}} + \frac{C_{Pb_{\alpha}}}{\rho_{Pb}}} \quad (7)$$

and

$$\rho_{\beta} = \frac{100}{\frac{C_{Sn_{\beta}}}{\rho_{Sn}} + \frac{C_{Pb_{\beta}}}{\rho_{Pb}}}, \quad (8)$$

where  $\rho_{\alpha}$  and  $\rho_{\beta}$  are the densities for each phase,  $C_{Sn_{\alpha}}$  and  $C_{Pb_{\alpha}}$  are the compositions of Sn and Pb in the  $\alpha$  phase,  $C_{Sn_{\beta}}$  and  $C_{Pb_{\beta}}$  are the compositions of Sn and Pb in the  $\beta$  phase, and  $\rho_{Sn}$  and  $\rho_{Pb}$  are the densities for Sn and Pb (Callister & Rethwisch, 2010, p. 97).

Using equations (7) and (8), with the values for the densities:  $\rho_{Sn} = 7.24$  and  $\rho_{Pb} = 11.23$  (g/cm<sup>3</sup>) (Callister & Rethwisch, 2010, p. 302) as well as the composition of the phases obtained from the phase diagrams from equation 1, the densities for each phases are obtained:

$$\rho_{\alpha} = \frac{100}{\frac{4}{7.24} + \frac{96}{11.23}} = 10.987783 \quad (9)$$

$$\rho_{\beta} = \frac{100}{\frac{99}{7.24} + \frac{1}{11.23}} = 7.265815 \quad (10)$$

From the values of the density of each phase and the fraction of the phases, the volume fraction can be calculated using equation (6):

$$V_\beta = \frac{\frac{W_\beta}{\rho_\beta}}{\frac{W_\alpha}{\rho_\alpha} + \frac{W_\beta}{\rho_\beta}} = \frac{\frac{0.589474}{7.265815}}{\frac{0.410526}{10.987783} + \frac{0.589474}{7.265815}} = 0.684686 \approx 0.68 \quad (11)$$

The volumen fraction of the primary phase is 0.68.

## 1.2

A Pb–25 at% Sn alloy was slowly cooled from 380°C to 50°C. Ideally, Sn phase is expected to precipitate within Pb-phase grains, but in reality, a eutectic structure appeared. Assuming there were no experimental issues such as weighing errors, discuss the reason why this phenomenon occurred.

**Sh:** Aca creo que deberia de ir la discusion del punto eutectico, pero ahorita no me acuerdo por que es que se forma esa cosa :c

## 2

### 2.1

Pure water was quasi-statically cooled from room temperature to  $-5^{\circ}\text{C}$  under 1 atm pressure. Calculate the critical nucleus radius under these conditions. Assume the nucleus is spherical, the latent heat is 6 kJ/mol, the interfacial energy between ice and water is 30 mJ/m<sup>2</sup>, and the density of ice is 1 g/cm<sup>3</sup>.

The critical nucleus radius can be calculated using the following equation:

$$r^* = \frac{-2\gamma}{\Delta G_v}, \quad (12)$$

where  $\gamma$  is the surface free energy, and  $\Delta G_v$  is the volume free energy change. Because  $\Delta G_v$  is a function of temperature:

$$\Delta G_v = \frac{\Delta H_f (T_m - T)}{T_m}. \quad (13)$$

Substituting equation 13 in 12 gives:

$$r^* = \left( \frac{-2\gamma T_m}{\Delta H_f} \right) \left( \frac{1}{T_m - T} \right), \quad (14)$$

where  $\gamma$  is the surface free energy in J/m<sup>2</sup>,  $\Delta H_f$  is the the latent heat of fusion in J/m<sup>3</sup>,  $T_m$  is the melting temperature in K and  $T$  is the transformation temperature in K (Callister & Rethwisch, 2010, p. 346-347).

Because the latent heat provided in the problem is given in kJ/mol, it is necessary to convert to J/m<sup>3</sup> for the calculation. Using the density of ice and the molar mass for water, 18.01528 g/mol:

$$\begin{aligned} \left( \frac{6000 \text{ J}}{\text{mol}} \right) \left( \frac{1 \text{ mol}}{18.01528 \text{ g}} \right) \left( \frac{1 \text{ g}}{\text{cm}^3} \right) \left( \frac{100 \text{ cm}}{1 \text{ m}} \right)^3 &= 333050610.370752 \text{ J/m}^3 \\ &\approx 3.33 \times 10^{-8} \text{ J/m}^3 \end{aligned} \quad (15)$$

Using equation 14, the critical nucleus radius can be calculated:

$$\begin{aligned} r^* &= \left( \frac{-2 * 0.03 * 273}{-333050610.370752} \right) \left( \frac{1}{273 - 268} \right) = 9.836342879999998 \times 10^{-9} \text{ m} \\ r^* &\approx 9.84 \times 10^{-9} \text{ m} \end{aligned} \quad (16)$$

The critical nucleus radius for water quasi-statically cooled from room temperature to  $-5^{\circ}$  is 9.84 nm.

## 2.2

**Explain how the critical nucleus radius changes if the pure water is further cooled, including the reason.**

To visualize the changes of the radius with further cooling water, the critical radius was calculated for different cooling temperatures, with a range of cooling temperatures of  $-5$  to  $-200^{\circ}\text{C}$ , using equation 14. The results were plotted in a graph, which is shown in figure 2:

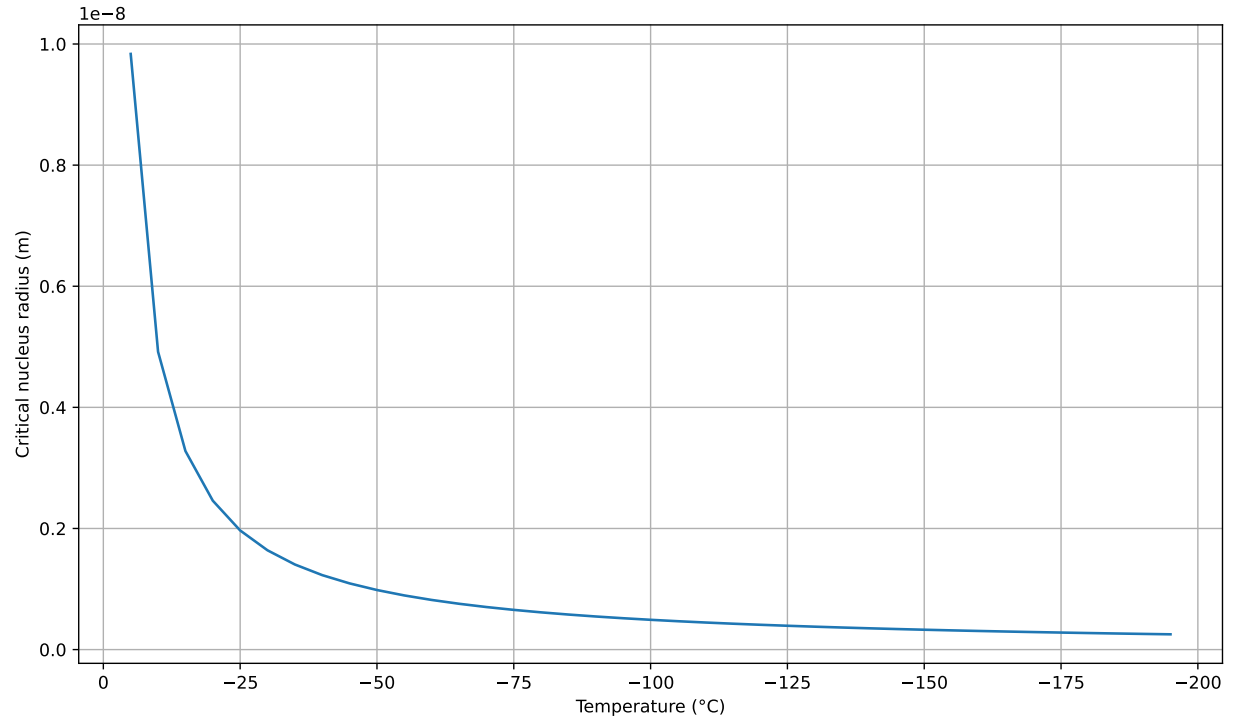


Figure 2: Critical nucleus radius as a function of temperature for water cooled in a range of temperature from  $-5$  to  $-200^{\circ}\text{C}$ .

*Source: Visualization by the author (code available at Cap Morales (2025))*

**Sh:** me falta explicar por que el radio cambia de esta manera

### 3

A specimen of pure aluminium was deformed and then heated to 500°C, resulting in recrystallization. Assuming the dislocation density of the deformed aluminium is  $10^{15} \text{ m}^{-2}$ , calculate the radius of the recrystallization nucleus. Assume the nucleus is spherical.

The critical nucleus size for recrystallization can be calculated with the following equation:

$$r_{crit} = \frac{2\gamma}{P}, \quad (17)$$

where  $P$  is the driving force for recrystallization in Pa and  $\gamma$  is the grain boundary energy in J/m<sup>2</sup> (Rollett, Rohrer, & Humphreys, 2017, p. 283).

The driving force  $P$  for recrystallization is provided by the dislocation density  $\rho$  which results in a stored energy, and it is given by:

$$P = \alpha \rho G b^2, \quad (18)$$

where  $\alpha$  is a constant of value 0.5,  $G$  is the shear modulus in Pa,  $b$  is the magnitude of the Burgers vector in m and  $\rho$  is the dislocation density in m<sup>-2</sup> (Rollett et al., 2017, p. 249).

The shear modulus ( $G$ ) value for Al is 25 GPa as it is shown in table 6.1 of Callister and Rethwisch (2010, p. 157).

The Burgers vector magnitude can be calculated from the Burgers vector, which for an FCC cell is given by:

$$\mathbf{b}(\text{FCC}) = \frac{a}{2} \langle uvw \rangle = \frac{a}{2} \langle 110 \rangle \quad (19)$$

(Callister & Rethwisch, 2010, p. 204).

The magnitude of the vector can be calculated using the following equation:

$$|\mathbf{b}| = \frac{a}{2} (u^2 + v^2 + w^2)^{1/2} = \frac{a}{2} (1^2 + 1^2 + 0^2)^{1/2} = \frac{a}{\sqrt{2}}, \quad (20)$$

where  $a$  is the lattice constant, and for Aluminum its value is: 0.40494 nm (Xu, Yamazaki, & Villars, 2011), which gives:

$$|\mathbf{b}| = \frac{0.40494}{\sqrt{2}} = 0.28633582. \quad (21)$$

Using the values of  $\alpha$ ,  $\rho$ ,  $G$ , and  $b$ , the value for the driving force can be calculated, using equation 18:

$$P = (0.5) (10^{15}) (25 \times 10^9) (0.28633582 \times 10^{-9})^2 = 10248525.225 \quad (22)$$

$$P \approx 10.2 \text{ MPa}$$

To calculate the critical nucleus size for recrystallization equation 17 is used, with the value of driving force ( $P$ ) and the value of the grain boundary energy of 375 mJ/m<sup>2</sup> (Rollett et al., 2017, p. 125):

$$\begin{aligned} r_{crit} &= \frac{2 * 0.375}{10248525.225} = 7.318126 \times 10^{-8} \text{m} \\ r_{crit} &\approx 73.1 \text{nm} \end{aligned} \tag{23}$$

The nucleus size of recrystallization for Aluminum is 73.1 nm.

## References

- Callister, W., & Rethwisch, D. (2010). *Materials science and engineering: An introduction*. Wiley.
- Cap Morales, S. N. (2025). *Github repository: Metallic materials*. [https://github.com/ShannonNCM/Metallic\\_materials/tree/main/Report2](https://github.com/ShannonNCM/Metallic_materials/tree/main/Report2). (Source code for data processing and visualization)
- Rollett, A., Rohrer, G., & Humphreys, J. (2017). *Recrystallization and related annealing phenomena*. Elsevier.
- Xu, Y., Yamazaki, M., & Villars, P. (2011). Inorganic materials database for exploring the nature of material. *Japanese Journal of Applied Physics*, 50(11S), 11RH02. doi: <https://doi.org/10.1143/jjap.50.11rh02>