**L2. Solidification of Metals**

*Find the critical radius of the nucleus and the number of atoms/nucleus for the homogeneous solidification of iron at following undercooling:   
10°C, 100°C, 200°C, 300°C, 400°C, 500°C and 600°C*

*Use the melting temperature of iron, 1538°C, the heat of fusion of 1737J/cm3 and the interfacial energy of 204x10-7J/cm2.*

*Note: iron crystallizes in BCC with 2atoms/cell and at high temperature has a lattice parameter of 0.286nm.*

*a. Create a plot undercooling vs. number of atoms/nucleus and debate on how undercooling would affect the size and morphology of the grains.*

*b. How would the number of atoms/nucleus change if iron would freeze first in a FCC lattice? Assume a lattice parameter of 0.3604nm.*

r\* = 2σTm/(ΔH\*ΔT) -> Critical radius

σ = 204 \* 10^-7 J/cm^3

Tm = 1538 °C = 1811 K

ΔH = 1737 J/cm^3

ΔT = {10°C, 100°C, 200°C, 300°C, 400°C, 500°C, 600°C}

Calculus example:

For ΔT = 100°C => r\* = 2\*204\*10^-7\*1811/1737\*100

r\* = 738888\*10^-7/173700 = 4.25\*10^-7 cm

N = Vnucleus / Vatom

Vnucleus = (4/3)\*π\*(r\*)^3

Vatom = a^3/Ncell

Vatom,BCC = (0.286\*10^-7)^3/2 = 1.17\*10^-24 cm^3

Vatom,FCC = (0.3604\*10^-7)^3/4 = 1.17\*10^-24 cm^3

=> confirm consistency

|  |  |  |  |
| --- | --- | --- | --- |
| ΔT [°C] | r\* [cm] | N BCC [atoms] | N FCC [atoms] |
| 10 | 4.25 \* 10^-6 | 2.76 \* 10^7 | 2.75 \* 10^7 |
| 100 | 4.25 \* 10^-7 | 2.76 \* 10^4 | 2.75 \* 10^7 |
| 200 | 2.13 \* 10^-7 | 3.45 \* 10^3 | 3.44 \* 10^3 |
| 300 | 1.42 \* 10^-7 | 1.02 \* 10^3 | 1.02 \* 10^3 |
| 400 | 1.06 \* 10^-7 | 4.31 \* 10^2 | 4.3 \* 10^2 |
| 500 | 8.51 \* 10^-8 | 2.21 \* 10^2 | 2.2 \* 10^2 |
| 600 | 7.09 \* 10^-8 | 1.28 \* 10^2 | 1.27 \* 10^2 |

As undercooling rises => critical radius increases

The no of atoms/nucleus decreases with the increase of the undercooling => more nucleation sites + finer grain structure

Low undercooling : large nuclei => coarse grain form

High undercooling : small nuclei => fine grains form due to rapid nucleation

The no of atoms/nucleus = slightly lower for FCC (larger lattice parameter)

The difference = minor => undercooling has a much stronger effect than the crystal structure.

High undercooling is used to refine grains in casting processes for better mechanical properties.