Primer Materials

Exercise 10

Spring 2021

Example 10.1

a) Natural shape of diamond crystals is octahedron. What face of diamond has the lowest surface energy?

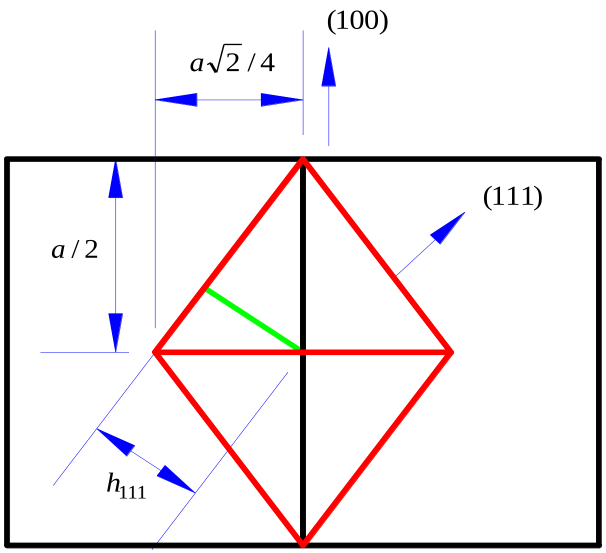
b) Is the following statement true : if a natural shape of a crystal is perfect cube (like sugar or NaCl), than the face (100) has the lowest surface energy? Why?

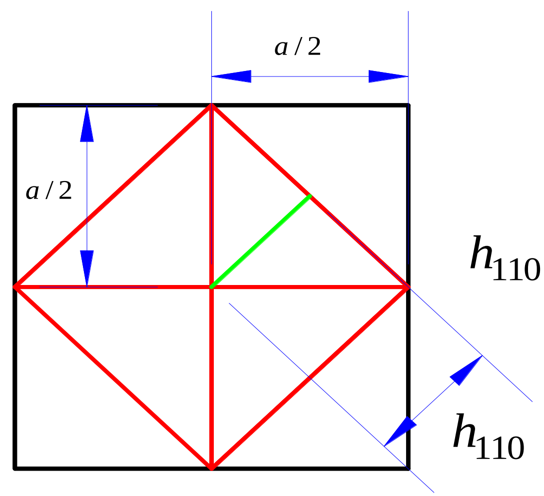
c) Estimate numerically the top limit on the ratio between the surface energy of diamond in the directions of (100), (110) and (111). Hint: consider an appropriate cross section of the unit cell and construct the Wolf's diagram.

a) There is only one family of planes in a cubic crystal that has eight members {1,1,1}. Therefore, the only face that can be the face of the octahedron crystal is {1,1,1}. Therefore, it has the lowest surface energy.

b) No, this is not true, because there are two families of planes that have six orthogonal members {1,0,0} and {1,1,0}. Therefore, if a crystal has a cubic shape it can be either way.

c) Consider cross section of the octahedron 1) parallel to its edge and be through it edges and 2) though its edges. Or, in the case of cubic crystal: $h_{hkl}=d_{hkl}/2=a/(2\cdot\sqrt{(h^2+k^2+l^2)})$





$$h_{110} = a\sqrt{2}/4$$

$$h_{111} = \frac{a}{2\sqrt{3}} \qquad \sigma_{111} < \frac{h_{111}}{h_{100}}\sigma_{100} = \sigma_{100}\frac{1}{2\sqrt{3}}\left(\frac{2}{1}\right) = \frac{\sigma_{100}}{\sqrt{3}}$$

$$\sigma_{111} < \frac{h_{111}}{h_{110}}\sigma_{110} = \sigma_{110}\frac{1}{2\sqrt{3}}\frac{4}{\sqrt{2}} = \sigma_{110}\frac{2}{\sqrt{6}}$$

$$\sigma_{111} < 0.588 \cdot \sigma_{100}$$

$$\sigma_{111} < 0.82 \cdot \sigma_{110}$$

Example 10.2

a) What is the attraction force between two silver particles having a shape of a cube with a side of 20 nm and separated by 10 nm gap. Plasma frequency of silver is 3.93 eV.

b) What is the energy of coagulation of 1 mole of silver consisting of these particles if they cannot approach each other closer than 0.15 nm. Consider that the final stage of coagulation yields a perfect cube built of these particles. Neglect the outer surface. Density of silver is 10.5 gm/cm^3, molar mass 108 gm/mol.

$$\omega_p^2 = \frac{ne^2}{m\varepsilon_0} \qquad \frac{F}{A} = -\frac{3}{124}\frac{\hbar\omega_p}{d^3}$$

There are 6 faces per one cubic particle and they approach each other from the distance of 10 nm to 0.15 nm.

$c := 3\cdot 10^{8}\cdot\frac{m}{s}$ $\quad \lambda := 12.9\cdot 10^{-6}\cdot m$ $\quad el := 1.6\cdot 10^{-19}\cdot C$ $\quad \varepsilon 0 := 8.85\cdot 10^{-14}\cdot\frac{F}{cm}$ $\quad eV := el\cdot V$

$Ep := 3.93\cdot eV$ $\quad d := 10\cdot 10^{-9}\cdot m$ $\quad a := 20\cdot 10^{-9}\cdot m$ $\quad d1 := 0.15\cdot 10^{-9}\cdot m$

$Mag := 108\cdot\frac{gm}{mole}$ $\quad \rho := 10.5\cdot\frac{gm}{cm^3}$

$Force := \frac{-3}{124}\cdot a^2\cdot\frac{Ep}{d^3}$ $\quad Force = -6.085\times 10^{-12} N$ $\quad Nfaces := 6\cdot\frac{Mag}{a^3\cdot\rho}$

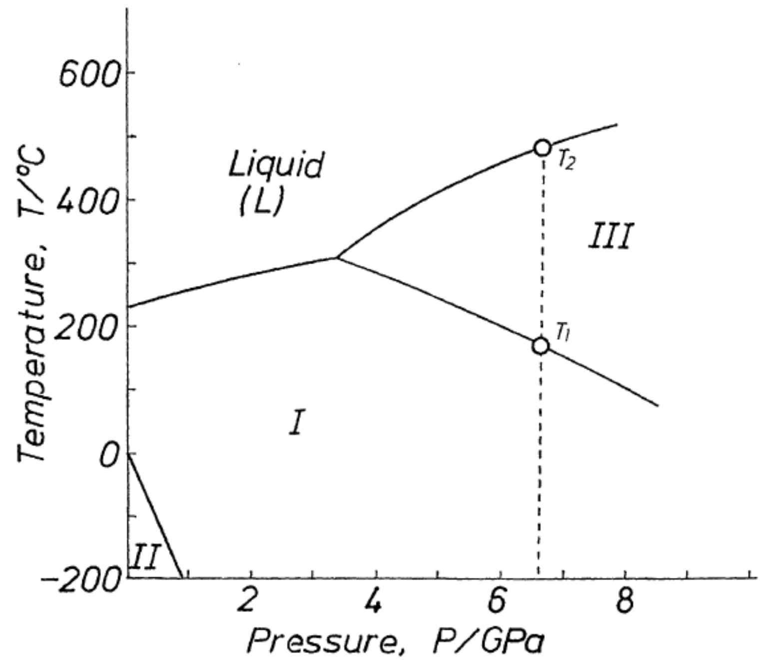
$$En\_per\_face := \int_{d}^{d1} Force\, dd$$

$$En := 3\cdot\frac{Mag}{a\cdot\rho}\cdot\left(\frac{-3}{124}\right)\cdot Ep\cdot\left(\frac{1}{d1^2}-\frac{1}{d^2}\right) \qquad \frac{En}{\frac{J}{mol}} = -1.043\times 10^{3}$$

It is clear that coagulation of metal nano-particles releases a lot of energy and without any special precaution they would coagulate..

Example 10.3

Calculate the size of the smallest particle of gray tin (phase II) that can exist (see the phase diagram). The surface tension of gray tin is ≈1 N/m



looking at the phase diagram, one can see that even at the lowest temperature, pressure of 1 GPa will cause the phase transition into phase I (white tin). Surface tension (Pascal pressure) will rich this value at $2\sigma/P=2$ nm