Advanced Construction Materials

Final exam

Name:

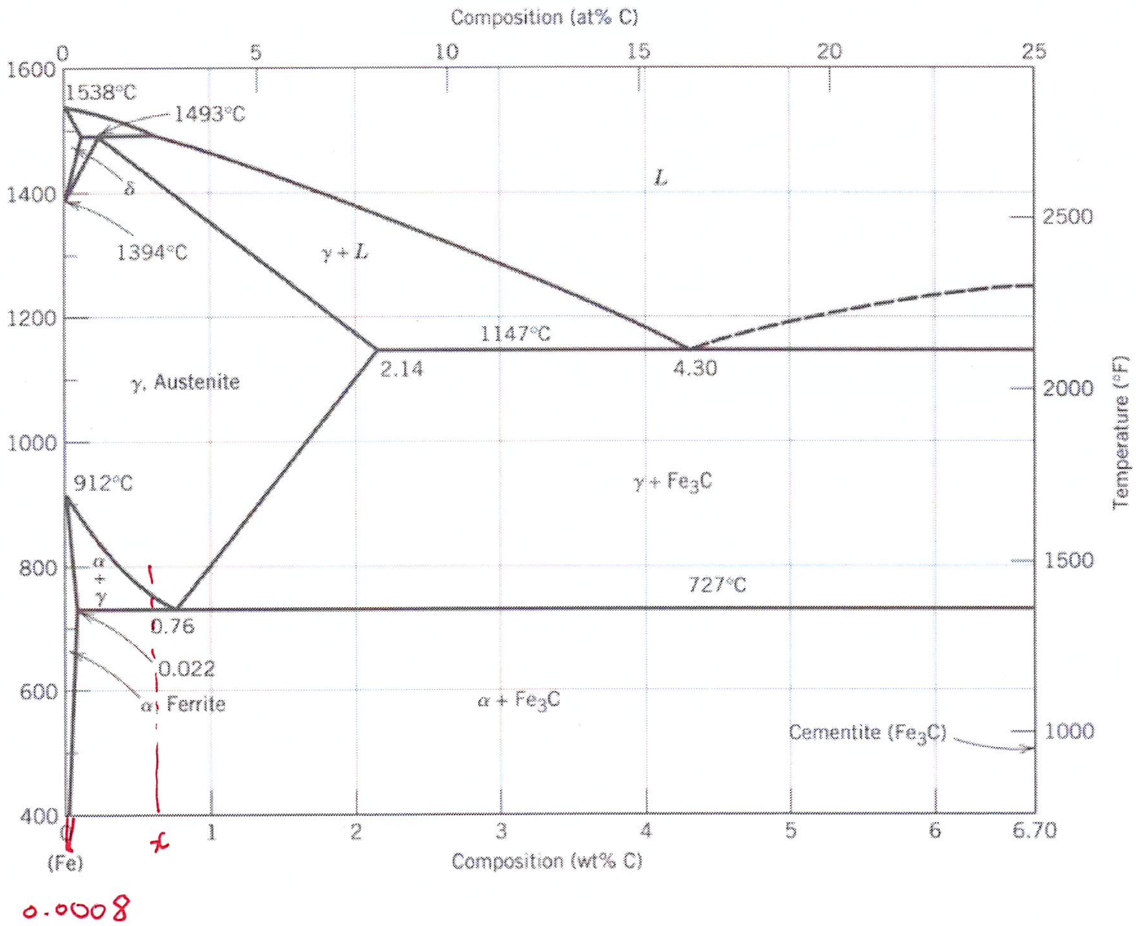
Student ID number:

(Total 100 points, 150 minutes)

Solution

Problem # 1 (10 pts)

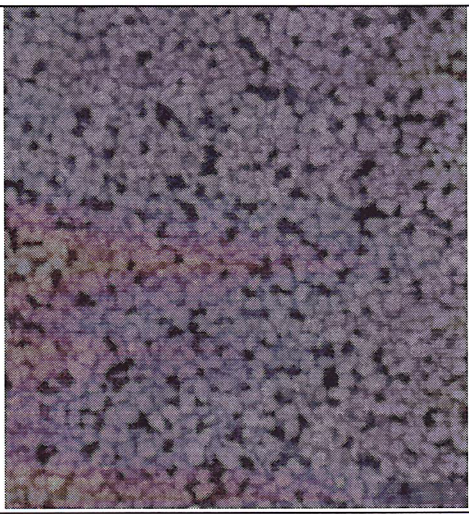
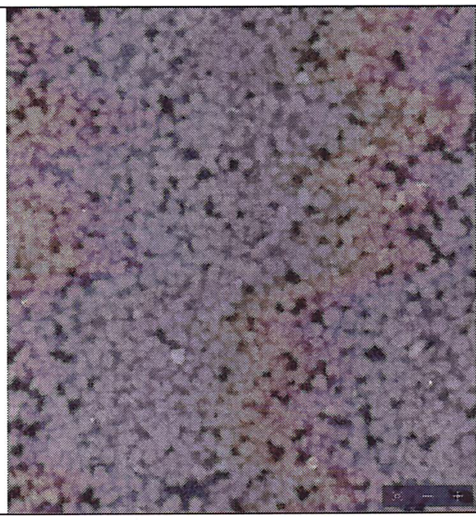
Design a plain-carbon steel alloy that contains 90 wt % ferrite and 10 wt % cementite at room temperature. Draw schematic microstructure of the steel alloy.



$$\frac{x - 0.0008}{6.67 - 0.0008} = 0.1 \quad ; \quad \underline{x = 0.67\,\%}$$

Problem # 2 (10 pts)

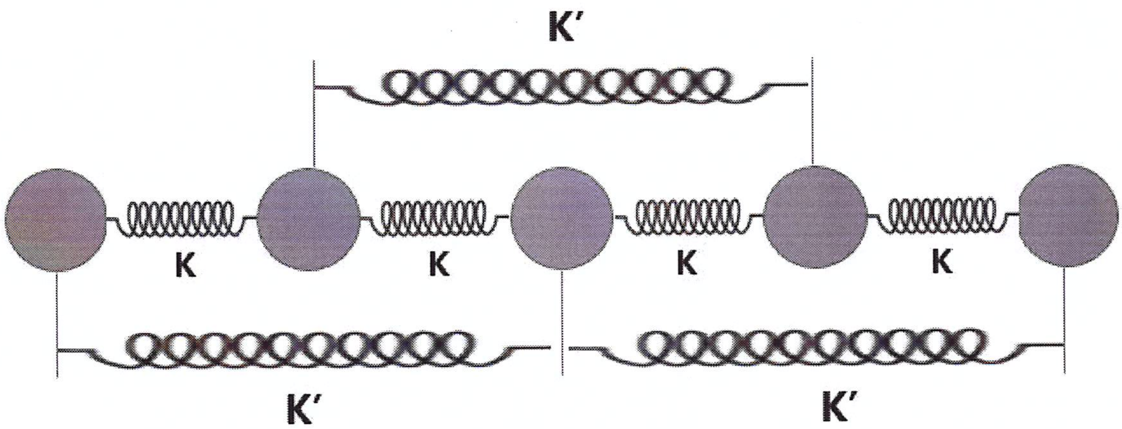
Below two images are obtained micro-tomographic sliced images of compacted sand (left) and improved sand with 5 wt % cement. Assuming you have a full stack of 2D images to be able to construct 3D structure of each samples, provide a detailed analysis strategy that you can suggest to study the impact of cement reinforcement on the sand. In your strategy, please include segmentation idea for this type of samples.

	
(left) Sand without cement	(right) Sand with 5 wt% cement reinforcement

- Transform to binary image using Otsu's method.
- Use segmentation method (such as Watershed) to segment cemented area from sand.
- or segment cemented area using other segmentation tool (e.g. malanobis distance)
- Do quantification to see the impact of cement on void structure between sand particles.

Problem # 3 (30 pts)

Consider a one dimensional lattice made up of a chain of identical atoms of mass m with a spacing a between neighboring atoms. Assume that the interatomic forces can be approximated by springs between nearest neighbor atoms and next-nearest neighbors atoms, with spring constants K and K′, respectively. Note, the nearest neighbors of site j are $j \pm 1$, while the second neighbors of site j are $j \pm 2$ (see below figure).



(a) Show that the vibration frequency of a mode with wavevector q is given by:

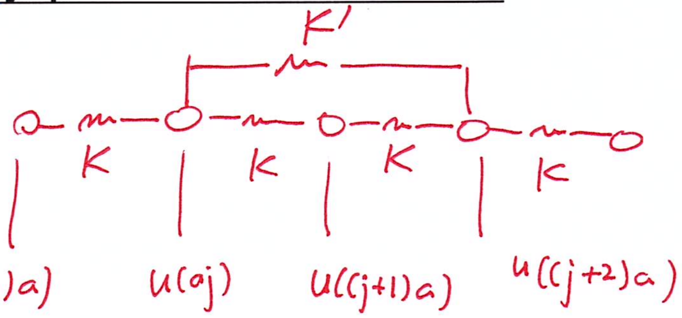
$$\omega_q^2 = \frac{2K}{m}\left(1-\cos qa\right)+\frac{2K'}{m}\left(1-\cos 2qa\right)$$

(b) By identifying the unit cell, discuss the allowed range of values for q. Find an expression for the velocity of the modes in the limit of small q.

(c) Explain why you always expect to get a zero frequency phonon mode when the wavevector approaches zero (i.e., $\omega_q \to 0$ as $q \to 0$)

Empty space

(a).



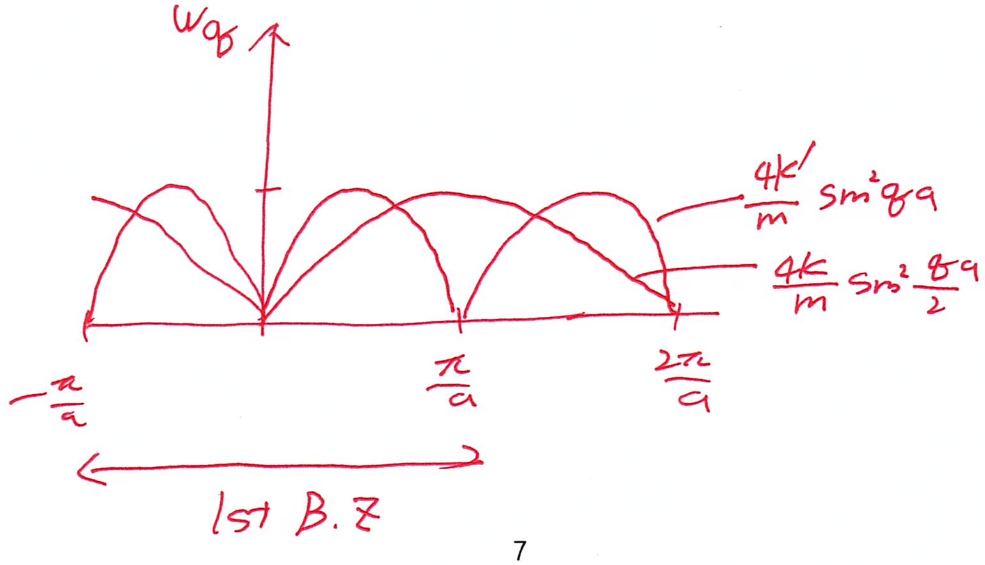
$$U_{nj} = U_0 e^{-i\omega t} e^{-kaj}$$

$$m\ddot{u}(aj) = K[u(aj+a)+u(aj-a)-2u(aj)]$$
$$+K'[u(aj+2a)+u(aj-2a)-2u(aj)]$$

$$-\omega^2 m = K\{e^{ika}+e^{-ika}-2\} + K'\{e^{ik2a}+e^{-ik2a}-2\}$$

$$\omega^2 = \frac{K}{m}(2-2\cos ka) + \frac{K'}{m}(2-2\cos 2ka)$$

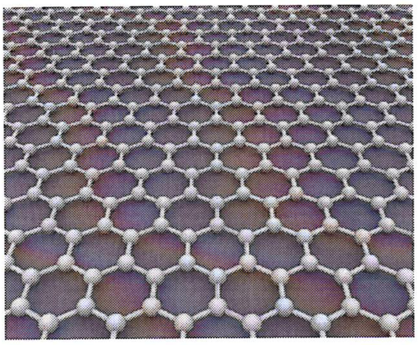
(b) $$\omega_q^2 = \frac{4K}{m}\sin^2\frac{qa}{2} + \frac{4K'}{m}\sin^2 qa$$



For small q ; $\cos(qa) \to 1-\frac{1}{2}(qa)^2$
$\cos(2qa) \to 1-\frac{1}{2}(2qa)^2$

Problem # 4 (30 pts)

Graphene forms a honeycomb lattice as shown in below figure. The distance between nearest atoms is l.

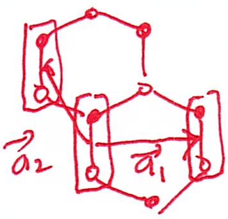


(a) Identify the Bravais lattice, basis atoms, and a pair of lattice vectors

(b) Find the reciprocal lattice vectors where you expect to see Bragg spots in X-ray diffraction. Work out the variation of X-ray scattering intensity for the different Bragg spots, by including the form factor that arises from the basis.

(c) In graphene l = 1.4Å, find the maximum wavelength X-ray one could use so that a Bragg reflection can occurs.

(a)



$\vec{a}_1 = \sqrt{3}\,l\,\hat{x}$

$\vec{a}_2 = -\frac{\sqrt{3}}{2} l\hat{x} + \frac{3}{2} l\hat{y}$

basis #1 $(0, \frac{l}{2})$

#2 $(0, -\frac{l}{2})$

(b) $\vec{b}_1 = \frac{4\pi}{3l}\left(\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}\right)$

$\vec{b}_2 = \frac{4\pi}{3l}\hat{y}$

$\vec{G} = m_1\vec{b}_1 + m_2\vec{b}_2 = \frac{2\sqrt{3}\pi}{3l} m_1\hat{x} + \frac{2\pi}{3l}(m_1 + 2m_2)\hat{y}$

$$S_G = \sum_j f_j e^{-i\vec{G}\cdot\vec{a}_j} \Big(\underbrace{e^{-i\vec{G}\cdot(0,\frac{l}{2})}}_{\text{basis \#1}} + \underbrace{e^{-i\vec{G}\cdot(0,-\frac{l}{2})}}_{\text{basis \#2}} \Big)$$

$$= 3f \cdot 2\cos\frac{\pi}{3}(m_1 + 2m_2)$$

Scattering intensity $\propto |S_G|^2$

(c) $\lambda = \frac{4\pi \sin\theta}{|G|}$ $\quad |G| = \frac{4\pi}{3l}(3m_1^2 + m_2^2)^{1/2}$

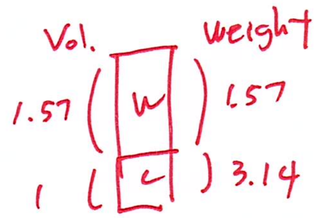
$m_1 = 0$ & $m_2 = 1 \Rightarrow \lambda = \frac{4\pi\sin\theta}{\frac{4\pi}{3l}} = 3l\sin\theta \Rightarrow \lambda_{max} = 3l$

Problem # 5 (10 pts)

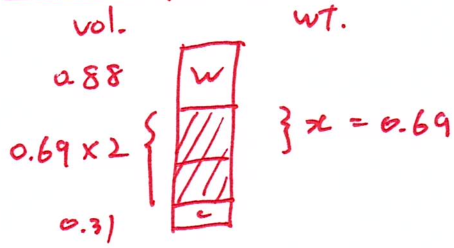
Calculate the bounds of Young's modulus of cement paste cured for specific days using Reuss-Voigt approximation. Use w/c ratio of 0.5, density of cement of 3.14 g/cm^3, Young's modulus of cement hydrates as 30 GPa. For chemically bound water (CBW) calculation, TGA was performed and result indicates that the value of CBW of "pre-dried" cement pastes after 14 days of curing is 18%. Assume the Young's modulus of unreacted cement particles and pores as zero.

$\frac{W}{C} = 0.5$; $\frac{V_w}{V_c \cdot 3.14} = 0.5$; if $V_c = 1$, $V_w = 1.57$

before hydration



after hydration



$\frac{x}{x + 3.14} = 18\%$; $x = 0.69$

$V_{void} = 0.88/2.57 = 34\%$

$V_{cement} = 0.31/2.57 = 12\%$

$V_{hydrate} = 1.38/2.57 = 54\%$

Reuss → $\frac{1}{E} = f_i \frac{1}{E_i}$; $E_{avg} = \underline{56\ GPa}$ //

Voigt → $E = f_i E_i$; $E_{avg} = \underline{16.\cancel{4}\ GPa}$ //

Problem # 6 (10 pts)

Show that the bulk modulus ($B \equiv v\left(\frac{\partial^2 u_{tot}}{\partial v^2}\right)$) for an ionic solid with NaCl structure (FCC) is given by

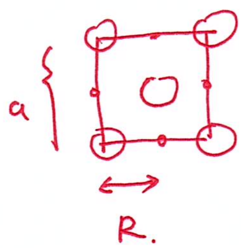
$$B = \frac{1}{18R_0}\left(\frac{d^2 u_{tot}}{dR^2}\right)_{R=R_0}$$

Where R_0 is the nearest neighbor distance in equilibrium.

If we use an equation of total energy for NaCl as a sum of repulsive energy of $U_{rep}(R) = C/R^4$ and attractive (coulomb) energy of $U_{att}(R) = -\alpha\frac{e^2}{4\pi\varepsilon R}$, derive different equation of bulk modulus for NaCl crystal.

$$B = v\left(\frac{\partial^2 U_T(R)}{\partial v^2}\right) \qquad v = \frac{1}{4}a^3 \quad 2R = a$$

$$= 2R^3$$



$$= 2R^3 \cdot \frac{\partial R}{\partial v} \cdot \frac{\partial}{\partial R}\left\{\frac{\partial R}{\partial v}\frac{\partial}{\partial R} U_T(R)\right\}$$

$$= 2R^3 \cdot \frac{1}{6R^2}\frac{\partial}{\partial R}\left\{\frac{1}{6R^2}\frac{\partial}{\partial R} U_t(R)\right\}$$

$$= \frac{R}{3}\left\{-\frac{1}{3R^2}\cancel{\frac{\partial}{\partial R}U_t(R)}^{\to 0} + \frac{1}{6R^2}\frac{\partial^2}{\partial R^2}U_t(R)\right\}$$

$$= \frac{1}{18R_0}\left(\frac{\partial^2 U_{TOT}(R)}{\partial R^2}\right)_{R=R_0} //$$

Empty space

- $U_T(R) = \dfrac{C}{R^4} - \dfrac{\alpha e^2}{4\pi\varepsilon R}$

$$\frac{\partial U_t(R)}{\partial R} = -4CR^{-5} + \frac{\alpha e^2}{4\pi\varepsilon R^2}$$

at $R = R_0$, $\dfrac{\partial U_t(R)}{\partial R} = 0$;

$$-4CR_0^{-5} + \frac{\alpha e^2}{4\pi\varepsilon R_0^2} = 0 \quad ; \quad \frac{4C}{R_0^5} = \frac{\alpha e^2}{4\pi\varepsilon R_0^2}$$

$$R_0^3 = \frac{16\pi C\varepsilon}{\alpha e^2}$$

$$R_0 = \left(\frac{16\pi C\varepsilon}{\alpha e^2}\right)^{1/3}$$

$$B = \frac{1}{18R_0}\left(\frac{\partial^2 U_{tot}(R)}{\partial R^2}\right)_{R=R_0}$$

$$= \frac{1}{18R_0}\left(20CR_0^{-6} - \frac{\alpha e^2}{2\pi\varepsilon R_0^3}\right)_{R_0}$$

Substitute R_0 into B.

$$B = \frac{20}{18}CR_0^{-7} - \frac{\alpha e^2}{36\pi\varepsilon R_0^4}$$

$$= \frac{10}{9}C\cdot\left(\frac{16\pi C\varepsilon}{\alpha e^2}\right)^{-7/3} - \frac{\alpha e^2}{36\pi\varepsilon}\left(\frac{16\pi C\varepsilon}{\alpha e^2}\right)^{-4/3}$$