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2018-31976

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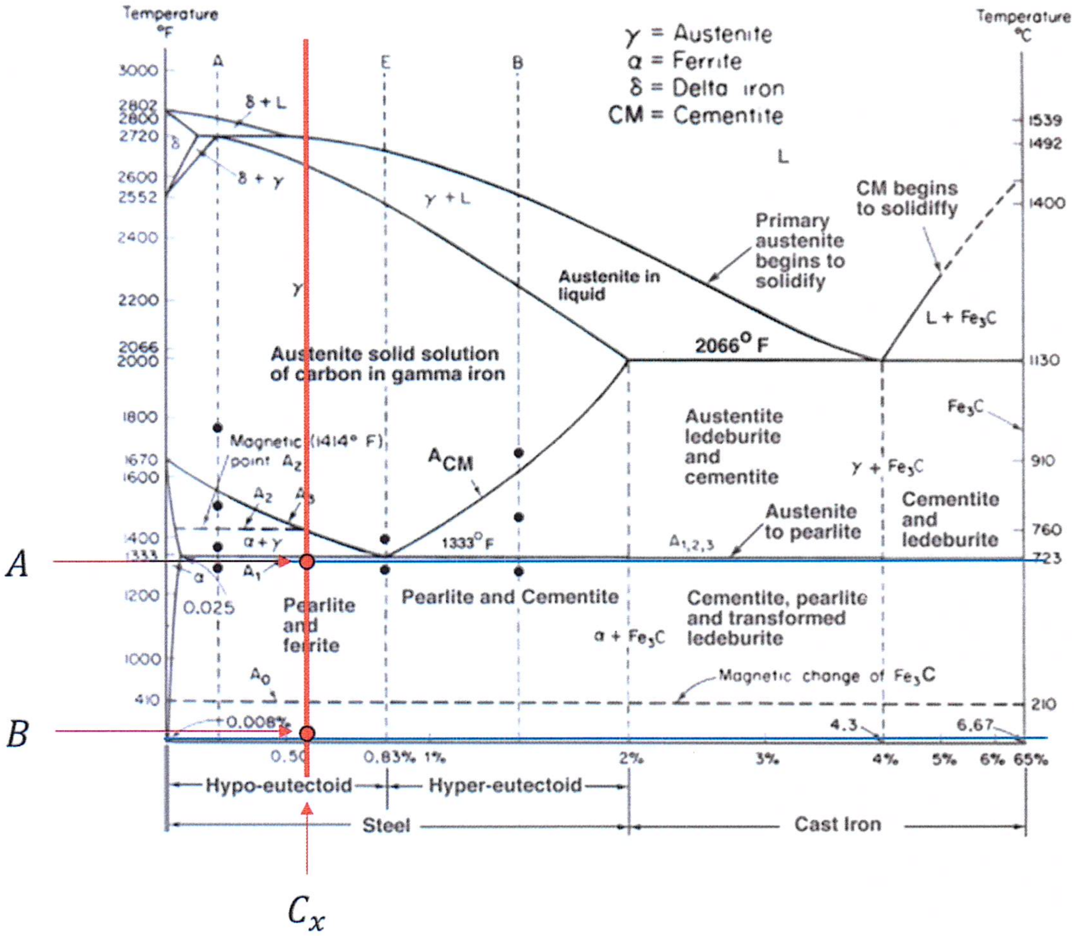
1. A hypoeutectoid plain-carbon steel that was slow-cooled from the austenitic region to room temperature contains 9.1 wt% eutectoid ferrite (ferrite in perlite). Assuming no change in structure on cooling from just below the eutectoid temperature to room temperature, what is the carbon content of the steel? **(20pt)**



i) Point A: $\alpha_A + \gamma_A$

$$\begin{cases} \alpha_A\% = \dfrac{0.8 - C_x}{0.8 - 0.025} \times 100 \\ \gamma_A\% = \dfrac{C_x - 0.025}{0.8 - 0.025} \times 100 \end{cases}$$

Here, α_A is proeutectoid ferrite and γ_A is Austenite.

ii) Point B: $\alpha_A + pearlite\left(\alpha_A + \begin{Bmatrix}\alpha_B \\ Fe_3C\end{Bmatrix}\right)$

$$\begin{cases} \alpha_{tot} = \alpha_A + \alpha_B = \dfrac{6.67 - C_x}{6.67 - 0.008} \times 100 \\ Fe_3C = \dfrac{C_x - 0.008}{6.67 - 0.008} \times 100 \end{cases} , \quad \alpha_B = 9.1\,[wt.\%] \text{ (eutectoid ferrite)}$$

From the above equation, the total amount of ferrite, which indicates that the summation of proeutectoid ferrite and eutectoid ferrite that is contained in the pearlite, can be calculated. Since the relative weight of eutectoid ferrite is given, the carbon content of steel can be obtained as below;

$$\frac{0.8 - C_x}{0.8 - 0.025} \times 100 + 9.1 = \frac{6.67 - C_x}{6.67 - 0.008} \times 100$$

$$\frac{6.67 - C_x}{6.662} - \frac{0.8 - C_x}{0.775} = 0.091$$

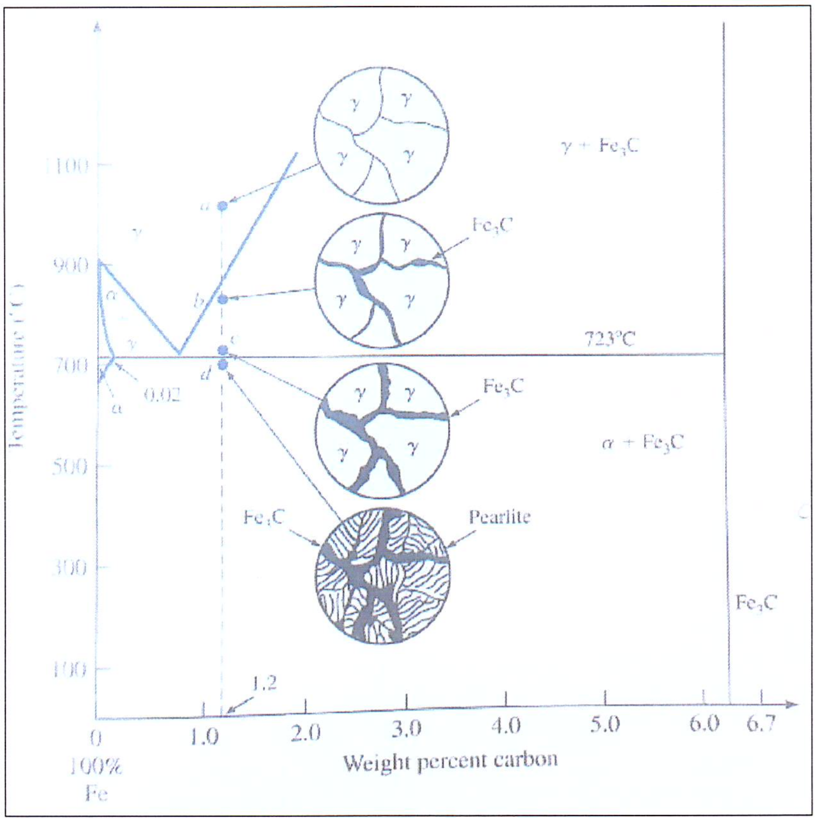
$$(6.67 - C_x) \times 0.775 - (0.8 - C_x) \times 6.662 = 0.091 \times 6.662 \times 0.775$$

$$5.887 C_x = 0.6302$$

$$C_x = 0.107\%$$

Therefore, the carbon content of steel is 0.107%.

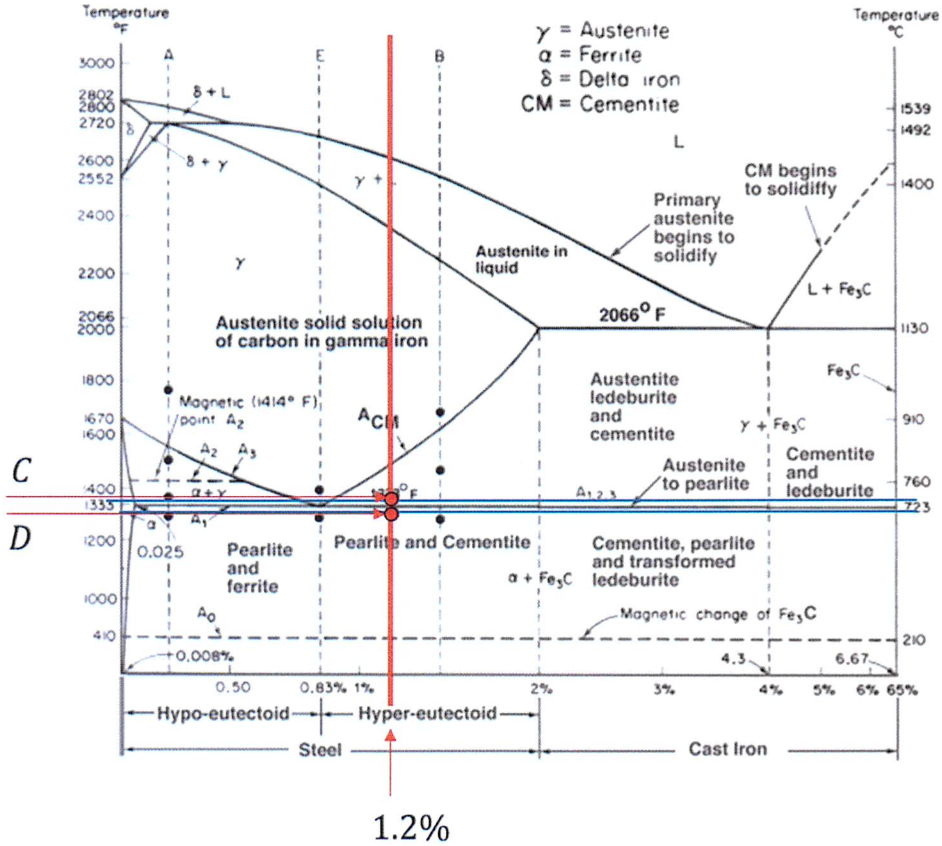
2. If a sample of a 1.2 percent C plain-carbon steel (hypereutectoid steel) is heated to about 950°C and held for a sufficient time, its structure will become essentially all austenite (point *a* in below Figure). With further slow cooling to point *c* of the Figure, which is just above 723°C, more proeutectoid cementite will be formed at the austenite grain boundaries. Calculate the weight percentage of the proeutectoid cementite at point *c* and *d*, respectively. **(20pt)**



i) Point C: $\gamma + (Fe_3C)_p$

$$\begin{cases} \gamma\% = \dfrac{6.67-1.2}{6.67-0.8}\times 100 = 93.19\% \\ (Fe_3C)_p\% = \dfrac{1.2-0.8}{6.67-0.8}\times 100 = 6.81\% \end{cases}$$

Here, $(Fe_3C)_p$ is proeutectoid cementite.



ii) Point D: $pearlite\ (\alpha + Fe_3C)$

Here, Fe_3C of pearlite is consisted of proeutectoid $(Fe_3C)_p$ and eutectoid $(Fe_3C)_e$, which is formed at the temperature just below 723°C. Therefore, the weight percentage of the proeutectoid cementite is same for both point C and D.

$\therefore$ Proeutectoid $Fe_3C\% = 6.81\%$

3. From LJ potential, interaction energy (u_{total}) between two atoms can be defined. In case of FCC structure, equation for bulk modulus (B) of FCC crystal can be formulated as below:

$$B = \frac{\sqrt{2}}{9R^*}\left(\frac{\partial^2 u_{tot}}{\partial R^2}\right)_{R^*}$$

Define the equation for a bulk modulus of BCC crystal. **(20pt)**

For a BCC structure, unit volume of atom can be calculated as below.

$$V = a^3, N = 2, R = \frac{\sqrt{3}}{2}a \rightarrow a = \frac{2}{\sqrt{3}}R$$

$$\therefore v = \frac{V}{N} = \frac{a^3}{2} = \frac{4}{3\sqrt{3}}R^3, \frac{\partial v}{\partial R} = \frac{4}{\sqrt{3}}R^2$$

$$P = -\frac{\partial U_{total}}{\partial V}$$

$$B = -V\left(\frac{\partial P}{\partial V}\right)\bigg|_{V=V^*} = V\left(\frac{\partial^2 U_{total}}{\partial V^2}\right)\bigg|_{V=V^*}$$

$$= Nv\left(\frac{\partial^2 U_{total}}{\partial V^2}\right)\bigg|_{V=V^*} \quad \left(\leftarrow V = Nv, \partial V = N\partial v, \partial V^2 = N^2 \partial v^2\right)$$

$$= Nv\left(\frac{\partial^2 U_{total}}{N^2 \partial v^2}\right)\bigg|_{V=V^*}$$

$$= v\left(\frac{\partial^2 \frac{U_{total}}{N}}{\partial v^2}\right)\Bigg|_{V=V^*} \quad \left(\leftarrow v = \frac{4}{3\sqrt{3}}R^3, \frac{U_{total}}{N} = u_{total}\right)$$

$$= \frac{4}{3\sqrt{3}}R^3 \frac{\partial^2 u_{total}}{\partial v^2}\bigg|_{R=R^*}$$

$$\frac{\partial(\ )}{\partial v} = \frac{\partial R}{\partial v}\frac{\partial(\ )}{\partial R} = \frac{\sqrt{3}}{4}\frac{1}{R^2}\frac{\partial(\ )}{\partial R}$$

$$\begin{aligned}
\frac{\partial^2(\ )}{\partial v^2} &= \left(\frac{\sqrt{3}}{4}\frac{1}{R^2}\frac{\partial(\ )}{\partial R}\right)\left(\frac{\sqrt{3}}{4}\frac{1}{R^2}\frac{\partial(\ )}{\partial R}\right) \\
&= \frac{\sqrt{3}}{4}\frac{1}{R^2}\left(-\frac{8\sqrt{3}R}{16R^4}\frac{\partial(\ )}{\partial R}\right) + \frac{\sqrt{3}}{4}\frac{1}{R^2}\left(\frac{\sqrt{3}}{4}\frac{1}{R^2}\right)\frac{\partial^2(\ )}{\partial R^2} \\
&= \frac{\sqrt{3}}{4}\frac{1}{R^2}\left(\frac{\sqrt{3}}{4}\frac{1}{R^2}\frac{\partial^2(\ )}{\partial R^2} - \frac{\sqrt{3}}{2}\frac{1}{R^3}\frac{\partial(\ )}{\partial R}\right)
\end{aligned}$$

$$\begin{aligned}
B &= \frac{4}{3\sqrt{3}}R^3\left.\frac{\partial^2 u_{total}}{\partial v^2}\right|_{R=R^*} \\
&= \frac{4}{3\sqrt{3}}R^3\frac{\sqrt{3}}{4}\frac{1}{R^2}\left.\left(\frac{\sqrt{3}}{4}\frac{1}{R^2}\frac{\partial^2 u_{total}}{\partial R^2} - \frac{\sqrt{3}}{2}\frac{1}{R^3}\frac{\partial u_{total}}{\partial R}\right)\right|_{R=R^*} \\
&= \frac{R^*}{3}\left(\frac{\sqrt{3}}{4}\frac{1}{R^{*2}}\left.\frac{\partial^2 u_{total}}{\partial R^2}\right|_{R=R^*} - \frac{\sqrt{3}}{2}\frac{1}{R^{*3}}\left.\frac{\partial u_{total}}{\partial R}\right|_{R=R^*}\right) \\
&= \frac{\sqrt{3}}{12R^*}\left.\frac{\partial^2 u_{total}}{\partial R^2}\right|_{R=R^*} \qquad \left(\because \left.\frac{\partial u_{total}}{\partial R}\right|_{R=R^*} = 0\right)
\end{aligned}$$

Therefore, the bulk modulus of BCC structure can be obtained as below.

$$\therefore B = \frac{\sqrt{3}}{12R^*}\left.\frac{\partial^2 u_{total}}{\partial R^2}\right|_{R=R^*}$$

✓

4. Jennite is a crystal that has similar nanostructure of C-S-H (main binding phase in cement paste). Crystal structure of Jennite is Triclinic which has 21 independent elastic constants (C_{ij}). Below is a list of the elastic constants (GPa unit) of Jennite published in *Moon et al. in Cement and Concrete Research 2015.*

C_{11}	100.0	C_{23}	41.7	C_{36}	− 1.4
C_{12}	49.0	C_{24}	3.0	C_{44}	23.3
C_{13}	46.6	C_{25}	− 4.9	C_{45}	− 3.2
C_{14}	− 6.7	C_{26}	− 6.9	C_{46}	1.8
C_{15}	4.9	C_{33}	78.8	C_{55}	27.0
C_{16}	− 3.0	C_{34}	0.3	C_{56}	− 0.6
C_{22}	127.5	C_{35}	− 6.0	C_{66}	41.1

Using the below two relations, calculate a bulk modulus of Jennite crystal. **(20pt)**

$$U = \frac{1}{2} B \cdot \delta^2$$ where δ is volumetric strain

$$U = \frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} C_{ij} e_i e_j$$ where $e_1 = e_2 = e_3 = \frac{1}{3}\delta$

$$\mathbf{C} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{bmatrix} = \begin{bmatrix} 100.0 & 49.0 & 46.6 & -6.7 & 4.9 & -3.0 \\ & 127.5 & 41.7 & 3.0 & -4.9 & -6.9 \\ & & 78.8 & 0.3 & -6.0 & -1.4 \\ & & & 23.3 & -3.2 & 1.8 \\ & & & & 27.0 & -0.6 \\ sym. & & & & & 41.1 \end{bmatrix}$$

For isotropic pressure condition,

$$e_1 = e_2 = e_3 = \frac{1}{3}\delta,\ e_4 = e_5 = e_6 = 0\,.$$

The above two relations about the elastic energy should be same each other.

$$\frac{1}{2} B \cdot \delta^2 = \frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} C_{ij} e_i e_j$$

$$
\begin{aligned}
U &= \frac{1}{2}\sum_{i=1}^{6}\sum_{j=1}^{6} C_{ij}e_i e_j \\
&= \frac{1}{2}\left(C_{11}e_1e_1 + C_{12}e_1e_2 + C_{13}e_1e_3 + C_{14}e_1e_4 + C_{15}e_1e_5 + C_{16}e_1e_6\right) \\
&\qquad + \ldots + \frac{1}{2}\left(C_{61}e_6e_1 + C_{62}e_6e_2 + C_{63}e_6e_3 + C_{64}e_6e_4 + C_{65}e_6e_5 + C_{66}e_6e_6\right) \\
&= \frac{1}{2}\left(C_{11}e_1e_1 + C_{12}e_1e_2 + C_{13}e_1e_3 + C_{21}e_2e_1 + C_{22}e_2e_2 + C_{23}e_2e_3 + C_{31}e_3e_1 + C_{32}e_3e_2 + C_{33}e_3e_3\right) \\
&= \frac{1}{2}\left(C_{11}e_1e_1 + C_{22}e_2e_2 + C_{33}e_3e_3 + 2C_{12}e_1e_2 + 2C_{13}e_1e_3 + 2C_{23}e_2e_3\right) \ (\because \textit{symmetry}) \\
&= \frac{1}{18}\delta^2\left(C_{11} + C_{22} + C_{33} + 2C_{12} + 2C_{13} + 2C_{23}\right) \\
&= \frac{580.9}{18}\delta^2\,[GPa]
\end{aligned}
$$

Therefore, the bulk modulus can be calculated as below.

$$
\begin{aligned}
&\frac{1}{2}B\cdot\delta^2 = \frac{580.9}{18}\delta^2 \\
&\therefore B = 64.54[GPa]
\end{aligned}
$$

5. Compute the bounds of effective moduli (bulk and shear modulus) for two-phase composite with different modulus contrast. The bulk modulus ratio of the inclusion and matrix in composite A is 10 : 1, and shear modulus ratio of 4:1, while in composite B, modulus contrast is much higher, where the bulk modulus ratio of inclusion and matrix is 100 : 1, and shear modulus ratio is 50 : 1. Use Poisson's ratio of the matrix as 0.1, if necessary.

   Compute the Reuss-Voigt bound and Hashin-Strikman bound for bulk and shear moduli as a function of volume fraction and discuss its result. **(20pt)**

$$\left(\frac{K_1}{K_2}\right)_A = 10,\ \left(\frac{G_1}{G_2}\right)_A = 4,\ \left(\frac{K_1}{K_2}\right)_B = 100,\ \left(\frac{G_1}{G_2}\right)_B = 50,\ \nu = 0.1$$

i) Reuss-Voigt bound

For the Reuss bound (lower bound), iso-stress situation is assumed. Then the average bulk modulus and the shear modulus can be obtained as below.

$$\hat{K}_R = \frac{\hat{P}}{\hat{\varepsilon}_v} = \frac{\hat{P}}{\sum f_i \cdot \varepsilon_{vi}} = \frac{\hat{P}}{\sum f_i \cdot \left(\frac{\hat{P}}{K_i}\right)} \quad \therefore \frac{1}{\hat{K}_R} = \sum \frac{f_i}{K_i}$$

$$\hat{G}_R = \frac{\hat{\tau}}{\hat{\gamma}} = \frac{\hat{\tau}}{\sum f_i \cdot \gamma_i} = \frac{\hat{\tau}}{\sum f_i \cdot \left(\frac{\hat{\tau}}{G_i}\right)} \quad \therefore \frac{1}{\hat{G}_R} = \sum \frac{f_i}{G_i}$$

where, f_i denotes the volume fraction

For the Voigt bound (upper bound), iso-strain situation is assumed.

$$\hat{K}_V = \frac{\hat{P}}{\hat{\varepsilon}_v} = \frac{\sum f_i \cdot P_i}{\hat{\varepsilon}_v} = \frac{\sum f_i \cdot (K_i \varepsilon_{vi})}{\hat{\varepsilon}_v} \quad \therefore \hat{K}_V = \sum f_i K_i$$

$$\hat{G}_V = \frac{\hat{\tau}}{\hat{\gamma}} = \frac{\sum f_i \cdot \tau_i}{\hat{\gamma}} = \frac{\sum f_i \cdot (G_i \gamma_i)}{\hat{\gamma}} \quad \therefore \hat{G}_V = \sum f_i G_i$$

ii) Hashin-Strikman bound

$$K_1 + \frac{f_2}{\frac{1}{K_2 - K_1} + \frac{f_1}{K_1 + \frac{4}{3}G_1}} \le \hat{K} \le K_2 + \frac{f_1}{\frac{1}{K_1 - K_2} + \frac{f_2}{K_2 + \frac{4}{3}G_2}}$$

$$G_1 + \frac{f_2}{\frac{1}{G_2 - G_1} + \frac{6(K_1 + 2G_1) f_1}{5(3K_1 + 4G_1) G_1}} \le \hat{G} \le G_2 + \frac{f_1}{\frac{1}{G_1 - G_2} + \frac{6(K_2 + 2G_2) f_2}{5(3K_2 + 4G_2) G_2}}$$

where, K_1 and G_1 are moduli of soft material, K_2 and G_2 are moduli of stiff material, respectively.

Set each modulus as below considering the ratio.

$$\begin{cases} (K_1)_A = 1,\ (K_2)_A = 0.1,\ (G_1)_A = 1,\ (G_2)_A = 0.25 \\ (K_1)_B = 1,\ (K_2)_B = 0.01,\ (G_1)_B = 1,\ (G_2)_B = 0.02 \end{cases}, \quad f_1 + f_2 = 1 \rightarrow f_2 = 1 - f_1$$

Then each bound for bulk and shear moduli can be plotted as a function of volume fraction.

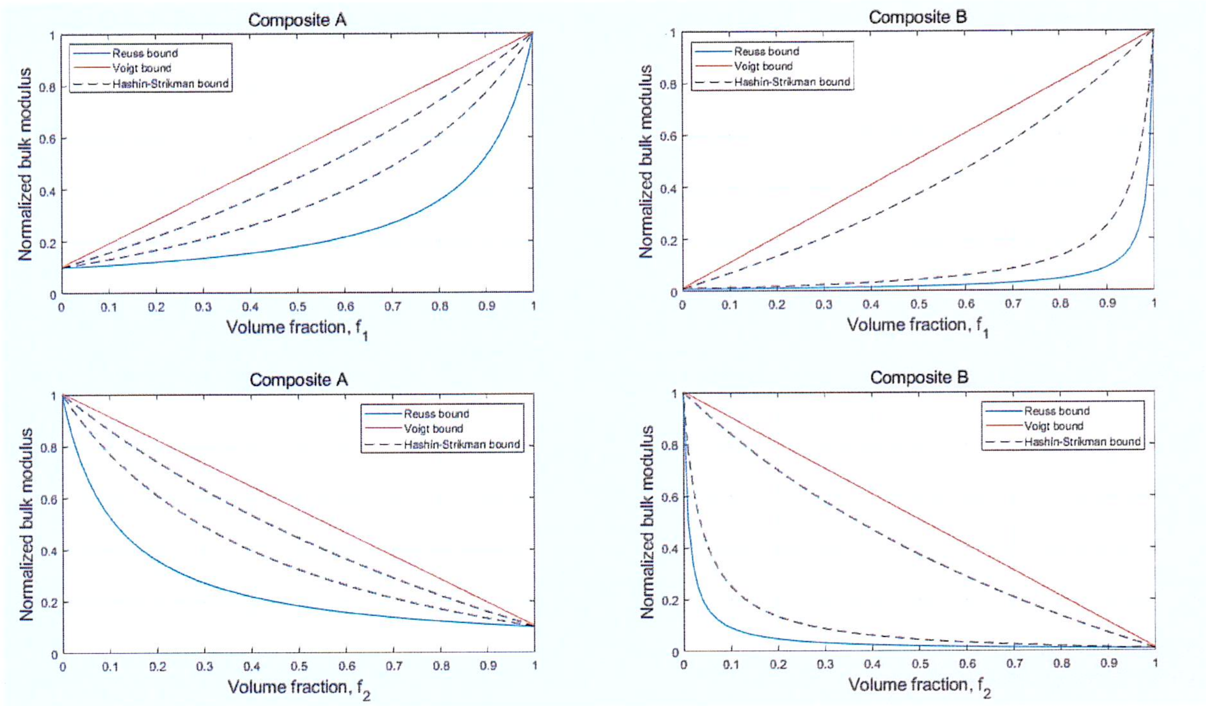


Figure 1 Normalized bulk modulus of each composite

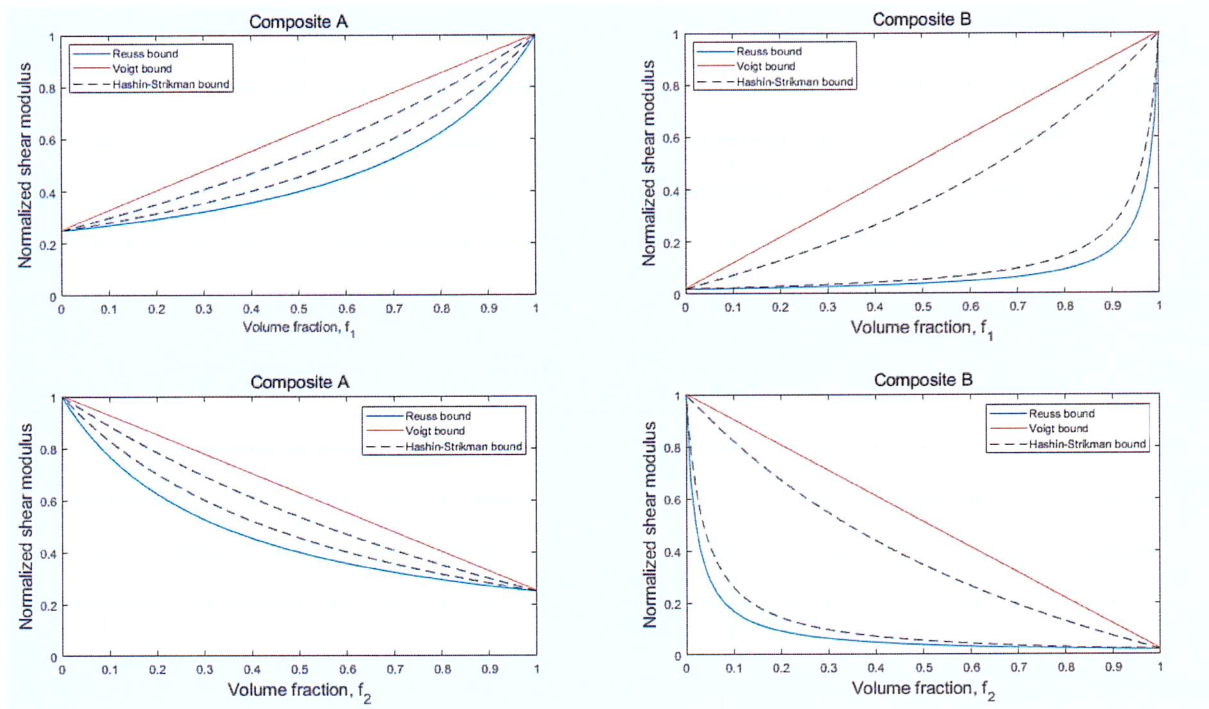


Figure 2 Normalized shear modulus of each composite

Although the composite material is consisted of several materials, the mechanical properties of the composite material do not show the average value of each mechanical properties. It presents different value along with the volume fraction of mixed materials.

Moreover, as shown in the above figure, Hashin-Strikman bound is more narrow than the Reuss-Voigt bound. This implies that the Hashin-Strikman bound allows to obtain more reliable mechanical properties of the composite materials. This is because that the Hashin-Strikman bound is derived from the spherical composite that is surrounded by another shell material, which is more realistic. On the other hand, the Reuss-Voigt bound is derived based on the iso-stress or iso- strain condition. This allows to obtain relatively accurate mechanical properties for fluid materials.

```
%% Advanced Construction Materials
% HW#4 - 5
% 2018-31976
% Kyoung-Min Kim
clc
clear

% Composite A
K1_A = 1;
K2_A = 0.1;
G1_A = 1;
G2_A = 0.25;

% Composite B
K1_B = 1;
K2_B = 0.01;
G1_B = 1;
G2_B = 0.02;

% Volume fraction
f1 = linspace(0,1,100)';
f2 = 1-f1;
%% Reuss-Voigt
% Reuss
KR_A = 1./(f1./K1_A+f2./K2_A);
GR_A = 1./(f1./G1_A+f2./G2_A);

KR_B = 1./(f1./K1_B+f2./K2_B);
GR_B = 1./(f1./G1_B+f2./G2_B);

% Voigt
KV_A = f1.*K1_A+f2.*K2_A;
GV_A = f1.*G1_A+f2.*G2_A;

KV_B = f1.*K1_B+f2.*K2_B;
GV_B = f1.*G1_B+f2.*G2_B;
%% Hashin-Strikman
% Lower bound
KHSL_A = K1_A+f2./(1./(K2_A-K1_A)+f1./(K1_A+(4/3)*G1_A));
GHSL_A = G1_A+f2./(1./(G2_A-
G1_A)+6*(K1_A+2*G1_A).*f1./(5*(3*K1_A+4*G1_A).*G1_A));

KHSL_B = K1_B+f2./(1./(K2_B-K1_B)+f1./(K1_B+(4/3)*G1_B));
GHSL_B = G1_B+f2./(1./(G2_B-
G1_B)+6*(K1_B+2*G1_B).*f1./(5*(3*K1_B+4*G1_B).*G1_B));
```

```
% Upper bound
KHSU_A = K2_A+f1./(1./(K1_A-K2_A)+f2./(K2_A+(4/3)*G2_A));
GHSU_A = G2_A+f1./(1./(G1_A-
G2_A)+6*(K2_A+2*G2_A).*f2./(5*(3*K2_A+4*G2_A).*G2_A));

KHSU_B = K2_B+f1./(1./(K1_B-K2_B)+f2./(K2_B+(4/3)*G2_B));
GHSU_B = G2_B+f1./(1./(G1_B-
G2_B)+6*(K2_B+2*G2_B).*f2./(5*(3*K2_B+4*G2_B).*G2_B));

%% Plots
% Bulk modulus
figure(1)
subplot(2,2,1)
plot(f1,KR_A)
hold on
grid on
plot(f1,KV_A)
plot(f1,KHSL_A,'k--')
plot(f1,KHSU_A,'k--')
xlabel('Volume fraction, f_{1}')
ylabel('Normalized bulk modulus')
title('Composite A')
legend('Reuss bound','Voigt bound','Hashin-Strikman bound')
axis([0,1,0,1])

subplot(2,2,2)
plot(f1,KR_B)
hold on
grid on
plot(f1,KV_B)
plot(f1,KHSL_B,'k--')
plot(f1,KHSU_B,'k--')
xlabel('Volume fraction, f_{1}')
ylabel('Normalized bulk modulus')
title('Composite B')
legend('Reuss bound','Voigt bound','Hashin-Strikman bound')
axis([0,1,0,1])


subplot(2,2,3)
plot(f2,KR_A)
hold on
grid on
plot(f2,KV_A)
plot(f2,KHSL_A,'k--')
plot(f2,KHSU_A,'k--')
xlabel('Volume fraction, f_{2}')
ylabel('Normalized bulk modulus')
title('Composite A')
legend('Reuss bound','Voigt bound','Hashin-Strikman bound')
axis([0,1,0,1])

subplot(2,2,4)
plot(f2,KR_B)
hold on
grid on
plot(f2,KV_B)
plot(f2,KHSL_B,'k--')
plot(f2,KHSU_B,'k--')
```

```
xlabel('Volume fraction, f_{2}')
ylabel('Normalized bulk modulus')
title('Composite B')
legend('Reuss bound','Voigt bound','Hashin-Strikman bound')
axis([0,1,0,1])

% Shear modulus
figure(2)
subplot(2,2,1)
plot(f1,GR_A)
hold on
grid on
plot(f1,GV_A)
plot(f1,GHSL_A,'k--')
plot(f1,GHSU_A,'k--')
xlabel('Volume fraction, f_{1}')
ylabel('Normalized shear modulus')
title('Composite A')
legend('Reuss bound','Voigt bound','Hashin-Strikman bound')
axis([0,1,0,1])

subplot(2,2,2)
plot(f1,GR_B)
hold on
grid on
plot(f1,GV_B)
plot(f1,GHSL_B,'k--')
plot(f1,GHSU_B,'k--')
xlabel('Volume fraction, f_{1}')
ylabel('Normalized shear modulus')
title('Composite B')
legend('Reuss bound','Voigt bound','Hashin-Strikman bound')
axis([0,1,0,1])

subplot(2,2,3)
plot(f2,GR_A)
hold on
grid on
plot(f2,GV_A)
plot(f2,GHSL_A,'k--')
plot(f2,GHSU_A,'k--')
xlabel('Volume fraction, f_{2}')
ylabel('Normalized shear modulus')
title('Composite A')
legend('Reuss bound','Voigt bound','Hashin-Strikman bound')
axis([0,1,0,1])

subplot(2,2,4)
plot(f2,GR_B)
hold on
grid on
plot(f2,GV_B)
plot(f2,GHSL_B,'k--')
plot(f2,GHSU_B,'k--')
xlabel('Volume fraction, f_{2}')
ylabel('Normalized shear modulus')
title('Composite B')
legend('Reuss bound','Voigt bound','Hashin-Strikman bound')
axis([0,1,0,1])
```