

Building Phase Diagram in Phase-Field Crystal Model

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1 Introduction

The following will go through the procedures needed to calculate phase equilibria when using the phase-field crystal model. We start with the pure material and then for a binary alloy. With these, it will be easy to generalize for any number of components.

It is worthwhile remembering that the phase diagram calculation is really a minimization problem. What I mean is that you are attempting to figure out what values or functional forms of your variables will allow your thermodynamic potential to be a minimum of the system, or in the case it is an entropic potential, a maximum of the system. Additionally, some of these variables can only minimize or maximize your potential under a constraint, for example for a pure material the constraint is constant number of atoms. It is these considerations that lead to the now recognized common tangent construction. Let us begin.

2 Single Component

1. Define free energy functional. For the specific model of the XPFC, the free energy functional can be written as

$$\mathcal{F} = \int d\mathbf{r} \left\{ \frac{n^2}{2} - \eta \frac{n^3}{6} + \chi \frac{n^4}{12} - \frac{n}{2} \int d\mathbf{r}' C(|\mathbf{r} - \mathbf{r}'|) n(\mathbf{r}') \right\} \quad (1)$$

Details can be found in several resources by Greenwood and coworkers.

2. Define structures of interest for the system. Define an *ansatz* (approximation) for how the density field is described. We know for bcc structures only a single wavelength, i.e., mode, is dominant, while for fcc we need two dominant length scales. For the liquid phase we know the amplitude is zero and is described solely by the average density.

$$n_{liq} = n_o \quad (2)$$

$$\begin{aligned}
n_{bcc} &= n_o + A_{110} \sum_j e^{-i\mathbf{k}_j \cdot \mathbf{r}} + \text{c.c.}, \quad \text{where } \mathbf{k}_j \text{ is reciprocal vectors} \\
&= n_o + 2A_{110} \left[\cos \left[k_o \frac{\sqrt{6}}{2} (x+y) \right] + \cos \left[k_o \frac{\sqrt{6}}{2} (x+z) \right] + \cos \left[k_o \frac{\sqrt{6}}{2} (y+z) \right] \right. \\
&\quad \left. + \cos \left[k_o \frac{\sqrt{6}}{2} (x-y) \right] + \cos \left[k_o \frac{\sqrt{6}}{2} (x-z) \right] + \cos \left[k_o \frac{\sqrt{6}}{2} (y-z) \right] \right] \quad (3)
\end{aligned}$$

$$\begin{aligned}
n_{fcc} &= n_o + A_{111} \sum_j e^{-i\mathbf{k}_j \cdot \mathbf{r}} + A_{200} \sum_j e^{-i\mathbf{q}_j \cdot \mathbf{r}} + \text{c.c.}, \quad \mathbf{k}_j, \mathbf{q}_j \text{ reciprocal vectors} \\
&= n_o + 2A_{111} (\cos[k_o(x+y+z)] + \cos[k_o(x-y+z)] + \cos[k_o(x+y-z)] + \cos[k_o(-x+y+z)]) \\
&\quad + 2A_{200} (\cos[2k_o x] + \cos[2k_o y] + \cos[2k_o z]) \quad (4)
\end{aligned}$$

where the dimensionless lattice spacings are $a_{bcc} = \sqrt{2/3}$ and $a_{fcc} = 1$ for the bcc and fcc respectively.

3. Substitute the density expansion into the free energy. Generate the free energies for the 3 phase for this system.

$$\mathcal{F}^{liq} = \int d\mathbf{r} \left\{ \frac{n_o^2}{2} - \eta \frac{n_o^3}{6} + \chi \frac{n_o^4}{12} - \frac{n_o}{2} \int d\mathbf{r}' C(|\mathbf{r} - \mathbf{r}'|) n_o(\mathbf{r}') \right\} \quad (5)$$

$$\mathcal{F}^{bcc} = \int d\mathbf{r} \left\{ \frac{n_{bcc}^2}{2} - \eta \frac{n_{bcc}^3}{6} + \chi \frac{n_{fcc}^4}{12} - \frac{n_{bcc}}{2} \int d\mathbf{r}' C(|\mathbf{r} - \mathbf{r}'|) n_{bcc}(\mathbf{r}') \right\} \quad (6)$$

$$\mathcal{F}^{fcc} = \int d\mathbf{r} \left\{ \frac{n_{fcc}^2}{2} - \eta \frac{n_{fcc}^3}{6} + \chi \frac{n_{fcc}^4}{12} - \frac{n_{fcc}}{2} \int d\mathbf{r}' C(|\mathbf{r} - \mathbf{r}'|) n_{fcc}(\mathbf{r}') \right\} \quad (7)$$

Note that the correlation function is chosen to be that which stabilizes the fcc structure.

4. Integrate over respective unit cell of the solid structures to get free energy densities, i.e., energy per unit volume.

$$f^{liq} = \frac{n_o^2}{2} - \eta \frac{n_o^3}{6} + \chi \frac{n_o^4}{12} - \frac{n_o^2}{2} \hat{C}(k_0) \quad (8)$$

$$\begin{aligned}
f^{bcc} &= \frac{n_o^2}{2} - \eta \frac{n_o^3}{6} + \chi \frac{n_o^4}{12} - \frac{n_o^2}{2} \hat{C}(k_0) \\
&\quad + (1 - \eta n_o + \chi n_o^2) 6A_{110}^2 - (\eta - 2\chi n_o) 8A_{110}^3 + 45\chi A_{110}^4 - 6A_{110}^2 \hat{C}(k_1)
\end{aligned} \quad (9)$$

$$\begin{aligned}
f^{fcc} &= \frac{n_o^2}{2} - \eta \frac{n_o^3}{6} + \chi \frac{n_o^4}{12} - \frac{n_o^2}{2} \hat{C}(k_0) + (1 - \eta n_o + \chi n_o^2) [4A_{110}^2 + 3A_{200}^2] \\
&\quad - (\eta - 2\chi n_o) 12A_{111}^2 A_{200} + 18\chi A_{111}^4 + \frac{15}{2} \chi A_{200}^4 48\chi A_{111}^2 A_{200}^2 \\
&\quad - 4A_{111}^2 \hat{C}(k_1) - 3A_{200}^2 \hat{C}(k_2) \quad (10)
\end{aligned}$$

where k_1 corresponds to the length scale of the $\{111\}$ family of planes, and k_2 corresponds to the $\{200\}$ family of planes for fcc.

5. Minimize for the amplitudes.

$$\begin{aligned}
A_{110}^{eq} &\longrightarrow \frac{\partial f^{bcc}}{\partial A_{110}} = 0 \\
A_{110}^{eq} &= \frac{1}{15} \frac{-2\chi n_o + \sqrt{-11\chi^2 n_o^2 + 11\chi\eta n_o + 15\chi\hat{C}(k_1) + \eta^2 - 15\chi + \eta}}{\chi} \quad (11)
\end{aligned}$$

$$\begin{aligned}
A_{111}^{eq} &\longrightarrow \frac{\partial f^{fcc}}{\partial A_{111}} = 0 \\
A_{200}^{eq} &\longrightarrow \frac{\partial f^{fcc}}{\partial A_{200}} = 0
\end{aligned} \tag{12}$$

For the fcc, it is difficult to solve for the system of equations for the two solutions of the amplitudes, often using maple the solutions turn out to be complex which is incorrect. So what we do is we assume that they follow a similar ratio that they have at $\sigma = 0$, and we rewrite the free energy in terms of this ratio for the $\{111\}$ amplitude. This is $A_{200} = .567795938323429 A_{111}$. Doing this and solving, we get

$$\begin{aligned}
A_{111}^{eq} = \frac{1}{\chi} &\left(-0.1491828941 \chi n_o + 0.07459144705 \eta + 0.2692662517 \left[-.6930453574 \chi^2 n_o^2 \right. \right. \\
&\left. \left. + .6930453574 \chi \eta n_o + .8052864347 \chi \hat{C}(k_1) + .1947135656 \chi \hat{C}(k_2) + 0.07673866066 \eta^2 - \chi \right]^{1/2} \right)
\end{aligned} \tag{13}$$

The important thing to note is that both equilibrium amplitudes now depend explicitly on the average density, the parameters of the model (η, χ) and the correlation parameters. And even though we made a crude approximation of the fcc, we still get some dependence on the variables through the simple ratio.

6. Substitute the equilibrium amplitude solutions into their respective free energies. The energies will now only depend on average density and the parameters of the model and **not the amplitudes**. The equations are too long to write here so I will just write them as functions and their dependents.

$$\tilde{f}^{liq}(n_o^\ell) = f^{liq}(n_o = n_o^\ell) \tag{14}$$

$$\tilde{f}^{bcc}(n_o^{bcc}) = f^{bcc}(n_o = n_o^{bcc}, A_{110} = A_{110}^{eq}) \tag{15}$$

$$\tilde{f}^{fcc}(n_o^{fcc}) = f^{fcc}(n_o = n_o^{fcc}, A_{111} = A_{111}^{eq}) \tag{16}$$

Note that for the fcc since we reduced it to one amplitude, it's the only amplitude we need to substitute back in. Keep in mind that if we ever needed the other amplitude, we just need to consider the ratio once again.

7. Now perform the common tangent construction. For the combinations of phase coexistence you might have, which in this system are, fcc-liquid, bcc-liquid, fcc-bcc, the following conditions should apply.

(a) fcc-liquid

$$\begin{aligned}
\mu_\ell &= \frac{\partial \tilde{f}^{liq}}{\partial n_o^\ell} & \mu_{fcc} &= \frac{\partial \tilde{f}^{fcc}}{\partial n_o^{fcc}} \\
&\text{or} \\
\mu_\ell &= \mu_{fcc} \equiv \mu_{eq}
\end{aligned} \tag{17}$$

$$\tilde{f}^{liq} - \mu_\ell(1 + n_o^\ell) = \tilde{f}^{fcc} - \mu_{fcc}(1 + n_o^{fcc}) \equiv P \tag{18}$$

where P is the pressure (or grand potential in the bulk phases), which should be the same in each phase.

(b) bcc-liquid

$$\begin{aligned}
\mu_\ell &= \frac{\partial \tilde{f}^{liq}}{\partial n_o^\ell} & \mu_{bcc} &= \frac{\partial \tilde{f}^{bcc}}{\partial n_o^{bcc}} \\
&\text{or} \\
\mu_\ell &= \mu_{bcc} \equiv \mu_{eq}
\end{aligned} \tag{19}$$

$$\tilde{f}^{liq} - \mu_\ell(1 + n_o^\ell) = \tilde{f}^{bcc} - \mu_{bcc}(1 + n_o^{bcc}) \equiv P \tag{20}$$

(c) fcc-bcc

$$\mu_{fcc} = \frac{\partial \tilde{f}^{fcc}}{\partial n_o^{fcc}} \quad \mu_{bcc} = \frac{\partial \tilde{f}^{bcc}}{\partial n_o^{bcc}}$$

or

$$\mu_{fcc} = \mu_{bcc} \equiv \mu_{eq} \quad (21)$$

$$\tilde{f}^{fcc} - \mu_\ell(1 + n_o^{fcc}) = \tilde{f}^{bcc} - \mu_{fcc}(1 + n_o^{bcc}) \equiv P \quad (22)$$

Note that in each of the different equilibrium cases you have as many equations as there are variables to be solved for. This is paramount.

If you follow these steps, and initialize the following parameters, $\eta = 1, \chi = 1$ as well with the correlation parameters $\hat{C}(k_0) = 0, k_1 = 2\sqrt{3}\pi$ (for $\{111\}$ family of planes), $k_2 = 4\pi$ (for $\{200\}$ family of planes), $\rho_{111} = 1, \beta_{111} = 8, \rho_{200} = 1$, and $\beta_{200} = 6$, then you should get a phase diagram like this one in FFig. 1.

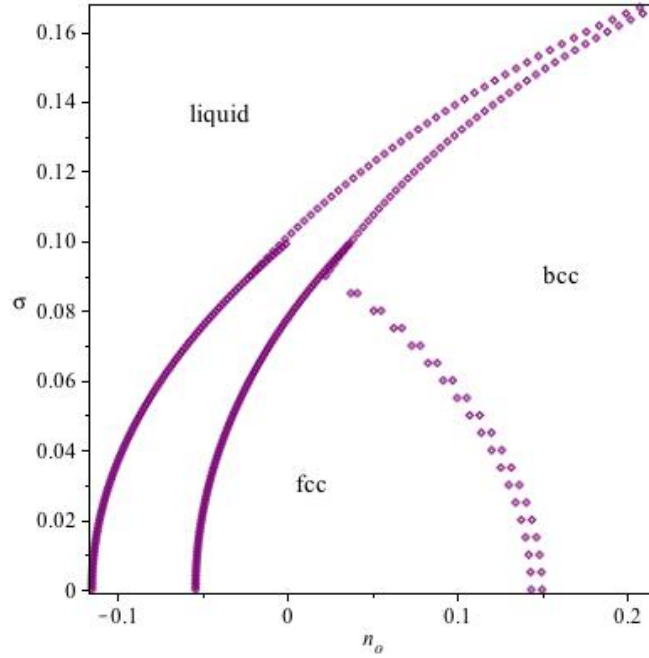


Figure 1: XPFC phase diagram, fcc-bcc-liquid. With $\eta = 1, \chi = 1, \hat{C}(k_0) = 0, k_1 = 2\sqrt{3}\pi, k_2 = 4\pi, \rho_{111} = 1, \beta_{111} = 8, \rho_{200} = 1$, and $\beta_{200} = 6$.

3 Single Component - Alternative Method

There is an alternative approach. Follow steps 1-4 like the above, and then go straight to this new step 5 that I have outlined below, which is the common tangent. However now the common tangent equations have an additional constraint which contributes additional equations for the minimization of the amplitudes. The following becomes the new common tangent construction.

5. New common tangent construction

(a) fcc-liquid

$$\frac{\partial f^{fcc}}{\partial A_{111}} = 0 \quad (23)$$

$$\frac{\partial f^{fcc}}{\partial A_{200}} = 0 \quad (24)$$

$$\begin{aligned} \mu_\ell &= \frac{\partial \tilde{f}^{liq}}{\partial n_o^\ell} & \mu_{fcc} &= \frac{\partial \tilde{f}^{fcc}}{\partial n_o^{fcc}} \\ \mu_\ell &= \mu_{fcc} \equiv \mu_{eq} \end{aligned} \quad (25)$$

$$\tilde{f}^{liq} - \mu_\ell(1 + n_o^\ell) = \tilde{f}^{fcc} - \mu_{fcc}(1 + n_o^{fcc}) \equiv P \quad (26)$$

where P is the pressure (or grand potential in the bulk phases), which should be the same in each phase.

(b) bcc-liquid

$$\frac{\partial f^{bcc}}{\partial A_{110}} = 0 \quad (27)$$

$$\begin{aligned} \mu_\ell &= \frac{\partial \tilde{f}^{liq}}{\partial n_o^\ell} & \mu_{bcc} &= \frac{\partial \tilde{f}^{bcc}}{\partial n_o^{bcc}} \\ \mu_\ell &= \mu_{bcc} \equiv \mu_{eq} \end{aligned} \quad (28)$$

$$\tilde{f}^{liq} - \mu_\ell(1 + n_o^\ell) = \tilde{f}^{bcc} - \mu_{bcc}(1 + n_o^{bcc}) \equiv P \quad (29)$$

(c) fcc-bcc

$$\frac{\partial f^{fcc}}{\partial A_{111}} = 0 \quad (30)$$

$$\frac{\partial f^{fcc}}{\partial A_{111}} = 0 \quad (31)$$

$$\frac{\partial f^{fcc}}{\partial A_{200}} = 0 \quad (32)$$

$$\begin{aligned} \mu_{fcc} &= \frac{\partial \tilde{f}^{fcc}}{\partial n_o^{fcc}} & \mu_{bcc} &= \frac{\partial \tilde{f}^{bcc}}{\partial n_o^{bcc}} \\ \mu_{fcc} &= \mu_{bcc} \equiv \mu_{eq} \end{aligned} \quad (33)$$

$$\tilde{f}^{fcc} - \mu_\ell(1 + n_o^{fcc}) = \tilde{f}^{bcc} - \mu_{fcc}(1 + n_o^{bcc}) \equiv P \quad (34)$$

We can now plot the first phase diagram with the one from this alternative method and this is shown in Fig. 2. The same parameters as with the above. Note that there is a difference between the two phase diagrams, but generally the phases are still in about the same places. This just showcases some of the inherent error associated with the approximation we made for the fcc amplitudes, since the bcc-liquid part has no noticeable differences.

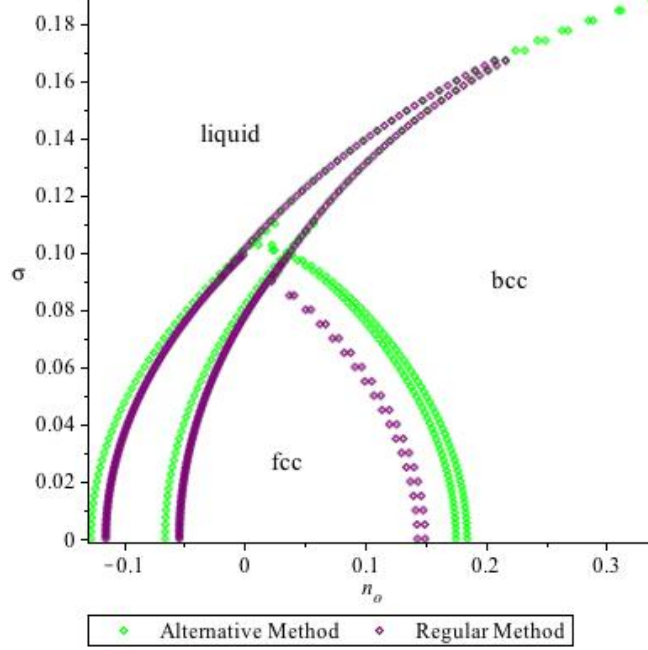


Figure 2: XPFC phase diagram, fcc-bcc-liquid. With $\eta = 1, \chi = 1, \hat{C}(k_0) = 0, k_1 = 2\sqrt{3}\pi, k_2 = 4\pi, \rho_{111} = 1, \beta_{111} = 8, \rho_{200} = 1$, and $\beta_{200} = 6$.

4 Two Components - Binary Alloy

1. The free energy for binary alloy has the form.

$$\mathcal{F} = \int d\mathbf{r} \left\{ \frac{n^2}{2} - \eta \frac{n^3}{6} + \chi \frac{n^4}{12} + \omega(n+1) \left[c \ln \frac{c}{c_r} + (1-c) \ln \frac{1-c}{1-c_r} \right] + \frac{\kappa^2}{2} |\nabla c|^2 - \frac{n}{2} \int d\mathbf{r}' C_{\text{eff}}(|\mathbf{r} - \mathbf{r}'|) n(\mathbf{r}') \right\} \quad (35)$$

where c_r is a reference composition and

$$C_{\text{eff}}(|\mathbf{r} - \mathbf{r}'|) = X_A(c) C^{AA}(|\mathbf{r} - \mathbf{r}'|) + X_B(c) C^{BB}(|\mathbf{r} - \mathbf{r}'|) \quad (36)$$

2. Define structures of interest for the system. For simplicity, let's use the same structures we used above for the pure material.

$$n_{liq} = n_o \quad (37)$$

$$\begin{aligned} n_{bcc} &= n_o + A_{110} \sum_j e^{-i\mathbf{k}_j \cdot \mathbf{r}} + \text{c.c.}, \quad \text{where } \mathbf{k}_j \text{ is reciprocal vectors} \\ &= n_o + 2A_{110} \left[\cos[k_o(x+y)] + \cos[k_o(x+z)] + \cos[k_o(y+z)] \right. \\ &\quad \left. + \cos[k_o(x-y)] + \cos[k_o(x-z)] + \cos[k_o(y-z)] \right] \end{aligned} \quad (38)$$

$$\begin{aligned} n_{fcc} &= n_o + A_{111} \sum_j e^{-i\mathbf{k}_j \cdot \mathbf{r}} + A_{200} \sum_j e^{-i\mathbf{q}_j \cdot \mathbf{r}} + \text{c.c.}, \quad \mathbf{k}_j, \mathbf{q}_j \text{ reciprocal vectors} \\ &= n_o + 2A_{111} (\cos[k_o(x+y+z)] + \cos[k_o(x-y+z)] + \cos[k_o(x+y-z)] + \cos[k_o(-x+y+z)]) \\ &\quad + 2A_{200} (\cos[2k_o x] + \cos[2k_o y] + \cos[2k_o z]) \end{aligned} \quad (39)$$

where the dimensionless lattice spacings are $a_{bcc} = 1$ and $a_{fcc} = 1$ for the bcc and fcc respectively.

3. Substitute the density expansion into the free energy. Generate the free energies for the 3 phase for this system.

$$\begin{aligned} \mathcal{F}^{liq} = \int d\mathbf{r} \left\{ \frac{n_o^2}{2} - \eta \frac{n_o^3}{6} + \chi \frac{n_o^4}{12} + \omega(n_o + 1) \left[c \ln \frac{c}{c_r} + (1 - c) \ln \frac{1 - c}{1 - c_r} \right] \right. \\ \left. + \frac{\kappa^2}{2} |\nabla c|^2 - \frac{n_o}{2} \int d\mathbf{r}' [X_A(c)C^{AA}(|\mathbf{r} - \mathbf{r}'|) + X_B(c)C^{BB}(|\mathbf{r} - \mathbf{r}'|)] n_o(\mathbf{r}') \right\} \end{aligned} \quad (40)$$

$$\begin{aligned} \mathcal{F}^{bcc} = \int d\mathbf{r} \left\{ \frac{n_{bcc}^2}{2} - \eta \frac{n_{bcc}^3}{6} + \chi \frac{n_{fcc}^4}{12} + \omega(n_{bcc} + 1) \left[c \ln \frac{c}{c_r} + (1 - c) \ln \frac{1 - c}{1 - c_r} \right] \right. \\ \left. + \frac{\kappa^2}{2} |\nabla c|^2 - \frac{n_{bcc}}{2} \int d\mathbf{r}' [X_A(c)C^{AA}(|\mathbf{r} - \mathbf{r}'|) + X_B(c)C^{BB}(|\mathbf{r} - \mathbf{r}'|)] n_{bcc}(\mathbf{r}') \right\} \end{aligned} \quad (41)$$

$$\begin{aligned} \mathcal{F}^{fcc} = \int d\mathbf{r} \left\{ \frac{n_{fcc}^2}{2} - \eta \frac{n_{fcc}^3}{6} + \chi \frac{n_{fcc}^4}{12} + \omega(n_{fcc} + 1) \left[c \ln \frac{c}{c_r} + (1 - c) \ln \frac{1 - c}{1 - c_r} \right] \right. \\ \left. + \frac{\kappa^2}{2} |\nabla c|^2 - \frac{n_{fcc}}{2} \int d\mathbf{r}' [X_A(c)C^{AA}(|\mathbf{r} - \mathbf{r}'|) + X_B(c)C^{BB}(|\mathbf{r} - \mathbf{r}'|)] n_{fcc}(\mathbf{r}') \right\} \end{aligned} \quad (42)$$

Note that there are now two separate correlation functions and they both enter all of the free energies.

4. Integrate over unit cells to attain energy densities.

$$\begin{aligned} f^{liq} = \frac{n_o^2}{2} - \eta \frac{n_o^3}{6} + \chi \frac{n_o^4}{12} + \omega(n_o + 1) \left[c \ln \frac{c}{c_r} + (1 - c) \ln \frac{1 - c}{1 - c_r} \right] \\ - \frac{n_o}{2} \left[X_A(c)\hat{C}^{AA}(k_0) + X_B(c)\hat{C}^{BB}(k_0) \right] \end{aligned} \quad (43)$$

$$\begin{aligned} f^{bcc} = \frac{n_o^2}{2} - \eta \frac{n_o^3}{6} + \chi \frac{n_o^4}{12} + \omega(n_o + 1) \left[c \ln \frac{c}{c_r} + (1 - c) \ln \frac{1 - c}{1 - c_r} \right] \\ + (1 - \eta n_o + \chi n_o^2) 6A_{110}^2 - (\eta - 2\chi n_o) 8A_{110}^3 + 45\chi A_{110}^4 - 6A_{110}^2 \hat{C}(k_1) \\ - \frac{n_o}{2} \left[X_A(c)\hat{C}^{AA}(k_0) + X_B(c)\hat{C}^{BB}(k_0) \right] - 6A_{110}^2 \left[X_A(c)\hat{C}^{AA}(k_1^{bcc}) + X_B(c)\hat{C}^{BB}(k_1^{bcc}) \right] \end{aligned} \quad (44)$$

$$\begin{aligned} f^{fcc} = \frac{n_o^2}{2} - \eta \frac{n_o^3}{6} + \chi \frac{n_o^4}{12} + \omega(n_o + 1) \left[c \ln \frac{c}{c_r} + (1 - c) \ln \frac{1 - c}{1 - c_r} \right] - \frac{n_o}{2} \left[X_A(c)\hat{C}^{AA}(k_0) + X_B(c)\hat{C}^{BB}(k_0) \right] \\ + (1 - \eta n_o + \chi n_o^2) [4A_{110}^2 + 3A_{200}^2] - (\eta - 2\chi n_o) 12A_{111}^2 A_{200} + 18\chi A_{111}^4 + \frac{15}{2} \chi A_{200}^4 48\chi A_{111}^2 A_{200}^2 \\ - 4A_{111}^2 \left[X_A(c)\hat{C}^{AA}(k_1^{fcc}) + X_B(c)\hat{C}^{BB}(k_1^{fcc}) \right] - 3A_{200}^2 \left[X_A(c)\hat{C}^{AA}(k_2^{fcc}) + X_B(c)\hat{C}^{BB}(k_2^{fcc}) \right] \end{aligned} \quad (45)$$

where k_1^{bcc} is the first mode of the bcc, while k_1^{fcc} and k_2^{fcc} are the first and second mode of the fcc.

5. Minimize for the amplitudes.

$$A_{110}^{eq} \longrightarrow \frac{\partial f^{bcc}}{\partial A_{110}} = 0 \quad (46)$$

$$A_{110}^{eq} = \frac{1}{15} \frac{-2\chi n_o + \sqrt{-11\chi^2 n_o^2 + 11\chi\eta n_o + 15\chi \left[X_A(c)\hat{C}^{AA}(k_1^{bcc}) + X_B(c)\hat{C}^{BB}(k_1^{bcc}) \right] + \eta^2 - 15\chi + \eta}}{\chi}$$

For the fcc, we again use the ratio of the amplitudes at $\sigma = 0$, from the pure material. This is $A_{200} = .567795938323429 A_{111}$.

$$A_{111}^{eq} \longrightarrow \frac{\partial f^{fcc}}{\partial A_{111}} = 0 \quad (47)$$

$$A_{111}^{eq} = \frac{1}{\chi} \left(-.1491828939\chi n_o + 0.07459144700\eta + \left[-0.6930453577\chi^2 n_o^2 + 0.6930453575\chi\eta n_o + 0.8052864344\chi \left[\hat{C}^{AA}(k_1^{fcc}) + X_B(c)\hat{C}^{BB}(k_1^{fcc}) \right] + 0.1947135656\chi \left[\hat{C}^{AA}(k_2^{fcc}) + X_B(c)\hat{C}^{BB}(k_2^{fcc}) \right] + 0.07673866067\eta^2 - \chi \right]^{1/2} \right) \quad (48)$$

Notice the concentration dependence that comes from the interpolation functions of the correlations. And not only do they depend on concentration, they also depend on the average density. As well they depend on the parameters of the model (η, χ) and the correlation parameters.

6. Substitute amplitudes and here we can assume that the average density is zero for all phases. Thermodynamically, this is assuming that there is no associated density jump between phases. The equations are again too long to write, so their dependencies will be highlighted.

$$\tilde{f}^{liq}(c^\ell) = f^{liq}(n_o = 0, c^\ell) \quad (49)$$

$$\tilde{f}^{bcc}(c^{bcc}) = f^{bcc}(n_o = 0, c^\ell, A_{110} = A_{110}^{eq}) \quad (50)$$

$$\tilde{f}^{fcc}(c^{fcc}) = f^{fcc}(n_o = 0, c^\ell A_{111} = A_{111}^{eq}) \quad (51)$$

Note again that the fcc only has one amplitude since we used the ratio.

7. Common tangent construction for the combinations of phases. These are fcc-liquid, bcc-liquid, fcc-bcc, t where we consider the following conditions

(a) fcc-liquid

$$\begin{aligned} \mu_\ell &= \frac{\partial \tilde{f}^{liq}}{\partial c^\ell} & \mu_{fcc} &= \frac{\partial \tilde{f}^{fcc}}{\partial c^{fcc}} \\ \text{or} \\ \mu_\ell &= \mu_{fcc} \equiv \mu_{eq} \end{aligned} \quad (52)$$

$$\tilde{f}^{liq} - \mu_\ell c^\ell = \tilde{f}^{fcc} - \mu_{fcc} c^{fcc} \equiv P \quad (53)$$

where P is the pressure (or grand potential in the bulk phases), which should be the same in each phase.

(b) bcc-liquid

$$\begin{aligned} \mu_\ell &= \frac{\partial \tilde{f}^{liq}}{\partial c^\ell} & \mu_{bcc} &= \frac{\partial \tilde{f}^{bcc}}{\partial c^{bcc}} \\ \text{or} \\ \mu_\ell &= \mu_{bcc} \equiv \mu_{eq} \end{aligned} \quad (54)$$

$$\tilde{f}^{liq} - \mu_\ell c^\ell = \tilde{f}^{bcc} - \mu_{bcc} c^{bcc} \equiv P \quad (55)$$

(c) fcc-bcc

$$\mu_{fcc} = \frac{\partial \tilde{f}^{fcc}}{\partial c^{fcc}} \quad \mu_{bcc} = \frac{\partial \tilde{f}^{bcc}}{\partial c^{bcc}}$$

or

$$\mu_{fcc} = \mu_{bcc} \equiv \mu_{eq} \quad (56)$$

$$\tilde{f}^{fcc} - \mu_{\ell} c^{fcc} = \tilde{f}^{bcc} - \mu_{fcc} c^{bcc} \equiv P \quad (57)$$

Each phase coexistence has as many equations as there are unknowns.

Follow the steps and set the following parameters, $\eta = 1.4, \chi = 1, \omega = 0.02, c_r = 0.5$ as well with the correlation parameters; bcc (\hat{C}^{BB}): $k_1^{bcc} = 2\sqrt{2}\pi, \rho_{110} = 1, \beta_{110} = 12, \alpha_{110} = 2$, fcc (\hat{C}^{AA}): $k_1^{fcc} = 2\sqrt{3}\pi, k_2^{fcc} = 4\pi, \rho_{111} = 1, \beta_{111} = 8, \alpha_{111} = 2, \rho_{200} = 1, \beta_{200} = 6$ and $\alpha_{200} = 2$. The phase diagram should look like Fig. 3.

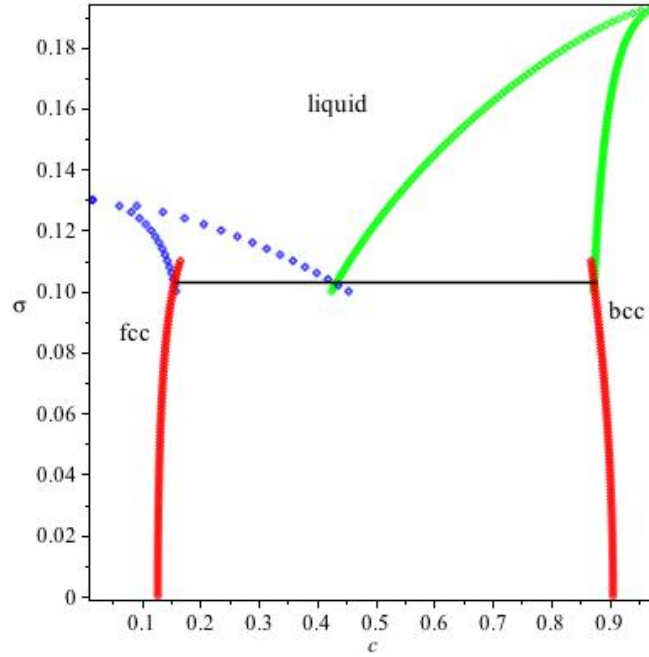


Figure 3: XPCF Eutectic phase diagram, fcc-bcc-liquid. With $\eta = 1.4, \chi = 1, \omega = 0.02, c_r = 0.5$ as well with the correlation parameters; bcc (\hat{C}^{BB}): $k_1^{bcc} = 2\sqrt{2}\pi, \rho_{110} = 1, \beta_{110} = 12, \alpha_{110} = 2$, fcc (\hat{C}^{AA}): $k_1^{fcc} = 2\sqrt{3}\pi, k_2^{fcc} = 4\pi, \rho_{111} = 1, \beta_{111} = 8, \alpha_{111} = 2, \rho_{200} = 1, \beta_{200} = 6$ and $\alpha_{200} = 2$.

You can also try the alternative method for the alloy phase diagram as well, but it is a little more involved so I did not include it here.