<u>Assignment 3:</u> Gibbs energy of AlNi phase (CsCl type) is modeled using two-sublattices as indicated below:

$$(\underline{AI},Ni)_{0.5}$$
:  $(AI,\underline{Ni})_{0.5}$ 

Calculate the site fractions of its sublattice constituents at 1200 K and 60 at. % of Ni. Write your program to do this. (Due date: 05-04-2018)

Given:

$$\begin{split} G_{\text{Al:Ni}}^{\text{AlNi}} &= +10083 - 4.813*T + \text{GHSERAL} \\ G_{\text{Ni:Ni}}^{\text{AlNi}} &= +8715.08 - 3.556*T + \text{GHSERNI} \\ G_{\text{Al:Ni}}^{\text{AlNi}} &= -56500 - 10.7*T + 1.4975*T*\ln(T) + 0.5*\text{GHSERAL} + 0.5*\text{GHSERNI} \\ G_{\text{Al:Ni}}^{\text{AlNi}} &= G_{\text{Ni:Al}}^{\text{AlNi}} \\ {}^{0}L_{\text{Al:Ni:Al}}^{\text{AlNi}} &= -14225 - 5.625*T \\ {}^{0}L_{\text{Al:Ni:Al,Ni}}^{\text{AlNi}} &= 0 L_{\text{Al:Ni:Al}}^{\text{AlNi}} \\ {}^{0}L_{\text{Al:Ni:Ni}}^{\text{AlNi}} &= -22050 \\ {}^{0}L_{\text{Al:Ni:Ni}}^{\text{AlNi}} &= 0 L_{\text{Ni:Al,Ni}}^{\text{AlNi}} \\ {}^{1}L_{\text{Ni:Al,Ni:Ni}}^{\text{AlNi}} &= 1115 \\ {}^{1}L_{\text{Al:Ni:Ni}}^{\text{AlNi}} &= 1 L_{\text{Ni:Al,Ni}}^{\text{AlNi}} \\ {}^{GHSERAL} &= -11278.4 + 188.684*T - 31.7482*T*\ln(T) - 1.231e + 028*T**(-9) \\ {}^{GHSERNI} &= -5179.16 + 117.854*T - 22.096*T*\ln(T) - 0.0048407*T**2 \end{split}$$