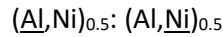


**Assignment 1:** Plot the lattice stability of hcp, fcc and liquid iron with respect to its bcc allotropic form. You may use PURE database from SGTE. – 5 marks (Due date: 17-02-2016)

**Assignment 2:** Plot the magnetic contribution to Gibbs energy of bcc iron as a function of temperature (300-1800 K) at 1 bar. Report enthalpy, entropy, heat capacity and Gibbs energy due to magnetic ordering of bcc iron at 400 K. What would be the most stable phase of iron at 400 K if it was not ferromagnetic? – 10 marks (Due date: 09-03-2016)

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



Calculate the site fractions of its sublattice constituents at 1200 K and 60 at. % of Ni. Write your program to do this. (Due date: 15-04-2016)

Given:

$$G_{\text{Al:Al}}^{\text{AlNi}} = +10083 - 4.813 \cdot T + \text{GHSERAL}$$

$$G_{\text{Ni:Ni}}^{\text{AlNi}} = +8715.08 - 3.556 \cdot T + \text{GHSERNI}$$

$$G_{\text{Al:Ni}}^{\text{AlNi}} = -56500 - 10.7 \cdot T + 1.4975 \cdot T \cdot \ln(T) + 0.5 \cdot \text{GHSERAL} + 0.5 \cdot \text{GHSERNI}$$

$$G_{\text{Al:Ni}}^{\text{AlNi}} = G_{\text{Ni:Al}}^{\text{AlNi}}$$

$${}^0 L_{\text{Al:Ni:Al}}^{\text{AlNi}} = -14225 - 5.625 \cdot T$$

$${}^0 L_{\text{Al:Al,Ni}}^{\text{AlNi}} = {}^0 L_{\text{Al,Ni:Al}}^{\text{AlNi}}$$

$${}^0 L_{\text{Ni:Al,Ni}}^{\text{AlNi}} = -22050$$

$${}^0 L_{\text{Al:Al,Ni}}^{\text{AlNi}} = {}^0 L_{\text{Al,Ni:Ni}}^{\text{AlNi}}$$

$${}^1 L_{\text{Ni:Al,Ni}}^{\text{AlNi}} = +1115$$

$${}^1 L_{\text{Al,Ni:Ni}}^{\text{AlNi}} = {}^1 L_{\text{Ni:Al,Ni}}^{\text{AlNi}}$$

$$\text{GHSERAL} = -11278.4 + 188.684 \cdot T - 31.7482 \cdot T \cdot \ln(T) - 1.231 \cdot 10^{28} \cdot T^{**}(-9)$$

$$\text{GHSERNI} = -5179.16 + 117.854 \cdot T - 22.096 \cdot T \cdot \ln(T) - 0.0048407 \cdot T^{**2}$$

**Assignment 4:** Given the following data on  $\Delta_{\text{mix}}H_{\text{m}}$  ( $\text{J. mol}^{-1}$ ) corresponding to the limiting binary systems of Ni-Ti-V-Zr, plot  $\Delta_{\text{mix}}H_{\text{m}}$  for  $\text{Nb}_{10}\text{Ti}_{30}\text{V}_{60-y}\text{Zr}_y$  from  $y=0$  to 60 at.% Zr using Muggianu, Colinet, and Kohler extrapolation methods (single plot with three curves, clearly marking each curve). Also report the numerical values of  $\Delta_{\text{mix}}H_{\text{m}}$  for an equiatomic quaternary alloy. (Due date: 22-04-2016)

System	$\Delta_{\text{mix}}H_{\text{m}}$
Nb-Ti	$x_{\text{Nb}}x_{\text{Ti}}(+3000)$
Nb-V	$x_{\text{Nb}}x_{\text{V}}(-1875)$
Nb-Zr	$x_{\text{Nb}}x_{\text{Zr}}(-10311+6709(x_{\text{Nb}}-x_{\text{Zr}}))$
Ti-V	$x_{\text{Ti}}x_{\text{V}}(+7600+2200(x_{\text{Ti}}-x_{\text{V}}))$
Ti-Zr	$x_{\text{Ti}}x_{\text{Zr}}(-968)$
V-Zr	$x_{\text{V}}x_{\text{Zr}}(-14900+3000x_{\text{Zr}}+1000x_{\text{Zr}}^2)$

**Assignment 5:** Using Thermo-Calc compute how the equilibrium partial pressures of the most dominant gas specie of a gas mixture, initially consisting of equimolar amounts of  $\text{SO}_3$  and  $\text{O}_2$ , vary as a function of temperature from 300 to 1500 K at 2 bar. You may use PSUB database. (Due date: 26-04-2016)