MM6010 - Assignment 3

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MM14B048

1 Question 1

The aim of this assignment is to calculate the site fractions of `Al` and `Ni` in `Al-Ni` system in B2 lattice. Let Y_1 be the fraction of site occupied by `Al` in the first sub lattice. Let Y_3 be the fraction of site occupied by `Ni` in the first sub lattice. Then, we have

$$Y_1 + Y_3 = 1 \tag{1}$$

Let Y_2 be the fraction of site occupied by `Al` in the second sub lattice. Let Y_4 be the fraction of site occupied by `Ni` in the second sub lattice. Then, we have

$$Y_2 + Y_4 = 1 \tag{2}$$

Further Y_1 and Y_2 can be related to the total composition of the alloy.

$$\frac{a_1 \times Y_1 + a_2 \times Y_2}{a_1 + a_2} = X_{Al} \tag{3}$$

Where,

X_{Al} is the overall composition of `Al` of the alloy,
a_1 is the number of sites of sub lattice 1 in the lattice,
a_2 is the number of sites of sub lattice 2 in the lattice,

Thus, the Gibbs energy of the system can be written in terms of only **one independent variable**(Y_1) . The Gibbs energy is then differentiated with respect to Y_1 and equated to zero, to find the Y_1 for which the **Gibbs energy is minimized**. The value obtained is checked to ensure that we have obtained a minima and not a maxima. The code given below implements this algorithm to find the site fractions of `Al` in different sub lattice.

```
clear all
clc


a1         = 0.5;
a2         = 0.5;
comp_of_al = 0.4;
Temp       = 1200;
R          = 8.314;

syms y1 % y1 = site fraction of Al in first sub lattice
syms y2 % y2 = site fraction of Al in second sub lattice
syms tot_gibbs % function to store the final gibbs lattice

y2 = (comp_of_al*(a1+a2) - a1*y1)/(a2); % Conservation of composition

%% Calculater the Gibbs_energy
Gibbs_ref =  y1*y2*G_Al_Al(Temp)                + ...
             (y1 + y2 -2*y1*y2)*G_Ni_Al(Temp)   + ...
             (1-y1)*(1-y2)*G_Ni_Ni(Temp);
% Calculate entropy contribution
G_config  = R*Temp*(a1*(y1*log(y1)+ (1-y1)*log(1-y1)) + ...
                                  a2*(y2*log(y2)+ (1-y2)*log(1-y2)));

% Calculate excess contribution
G_e       = y2*(1-y2)*y1*(L_0_Al__Al_Ni(Temp)           + ...
```

```
                                                L_1_Al__Al_Ni(Temp)*(2*y2-1));
G_e       = G_e + y2*(1-y2)*(1-y1)*(L_0_Ni__Al_Ni(Temp) + ...
                                                L_1_Ni__Al_Ni(Temp)*(2*y2-1));
G_e       = G_e + y1*(1-y1)*y2*(L_0_Al_Ni__Al(Temp)     + ...
                                                L_1_Al_Ni__Al(Temp)*(2*y1-1));
G_e       = G_e + y1*(1-y1)*(1-y2)*(L_0_Al_Ni__Ni(Temp) + ...
                                                L_1_Al_Ni__Ni(Temp)*(2*y1-1));


Gibbs_tot = Gibbs_ref + G_config + G_e;
% Find y1 that gives the minimum Gibbs
tot_gibbs = symfun((diff(Gibbs_tot,y1)),y1);
gibbs_double_diff = diff(tot_gibbs,y1);
tot_gibbs = symfun(simplify(tot_gibbs),y1);
total_gibbs = matlabFunction(tot_gibbs);
options = optimoptions('fsolve','FunctionTolerance',1E-12,'StepTolerance',1E-12);
S = fsolve(total_gibbs,0.000005,options);
gibbs_double_diff = diff(tot_gibbs,y1);
%% Print the Output
y1 = S;
if(subs(gibbs_double_diff)) > 0
    disp ('You have reached a minima');
else
    disp ('You have reached a maxima, change the initial value to reach a minima')
    ;
end
y2 = (comp_of_al*(a1+a2) - a1*y1)/(a2);
X = ['Site fraction of Al in 1st sublattice = ',num2str(y1)];
disp(X);
X = ['Site fraction of Al in 2nd sublattice = ',num2str(y2)];
disp(X);

%% Function definitions for different parameters

function y = GHSERAL(T)
y = -11278.4 + 188.684*T - 31.7482*T*log(T) - 1.231e+028*(T^( - 9));
end

function y = GHSERNI(T)
y = -5179.16+117.854*T - 22.096*T*log(T) -0.0048407*T^2;
end

function y = G_Al_Al(T)
y=10083-4.813*T+GHSERAL(T);
end

function y = G_Ni_Ni(T)
y=8715.08-3.556*T + GHSERNI(T);
end

function y =G_Ni_Al(T)
y=-56500-10.7*T +1.4975*T*log(T)+0.5*GHSERAL(T)+0.5*GHSERNI(T);
end



function y = L_0_Al_Ni__Ni(~)
y = -22050;
end
function y = L_1_Al_Ni__Ni(~)
y = 1115;
end
function y = L_0_Al_Ni__Al(T)
y = -14225-5.625*T;
end
function y = L_1_Al_Ni__Al(~)
```

```
y = 0.0;
end
function y = L_0_Ni__Al_Ni(~)
y = -22050;
end
function y = L_1_Ni__Al_Ni(~)
y = 1115;
end
function y = L_0_Al__Al_Ni(T)
y = -14225-5.625*T;
end
function y = L_1_Al__Al_Ni(~)
y = 0.0;
end
```

The output of the above code is given below.

```

Equation solved.

fsolve completed because the vector of function values is near zero
as measured by the default value of the function tolerance, and
the problem appears regular as measured by the gradient.

<stopping criteria details>

You have reached a minima
Site fraction of Al in 1st sublattice = 1.3026e-05
Site fraction of Al in 2nd sublattice = 0.79999
```

This value might be an artefact due to the numerical errors. Since, the value of `ln()` blows up nearer to zero, the numerical evaluation of those functions is prone to errors and they may manifest in the final answer as well.