
```

1;

% constants (no independent composition variable)
R=8.314;
T=1200;
x_Ni=0.6;
x_Al=1-x_Ni;
a1=0.5;
a2=0.5;

% to find (one independent site fraction)
% y_Al_1=0.1;
syms y_Al_1;

y_Al_2=(x_Al-a1*y_Al_1)/a2;
y_Ni_1=(1-y_Al_1);
y_Ni_2=(x_Ni-a1*y_Ni_1)/a2;

% since the number of independent site fractions is not the
% same as the number of independent mole fractions,
% we must use G minimisation to get the site fractions.

G_SER_Al=(-1)*11278.4+188.684*T-31.7482*T*log(T)-1.231e+028*T^(-9);
G_SER_Ni=(-1)*5179.16+117.854*T-22.096*T*log(T)-0.0048407*T^2;
G_Al_Al=10083-4.813*T+G_SER_Al;
G_Ni_Ni=8715.08-3.556*T+G_SER_Ni;
G_Al_Ni=(-1)*56500-10.7*T+1.4975*T*log(T)+(0.5)*(G_SER_Al+G_SER_Ni);

G_ref=y_Al_1*y_Al_2*G_Al_Al+y_Ni_1*y_Ni_2*G_Ni_Ni+...
(y_Al_1*y_Ni_2+y_Ni_1*y_Al_2)*G_Al_Ni;

G_conf=R*T*(0.5)*(y_Al_1*log(y_Al_1)*y_Al_2*log(y_Al_2)...
+y_Ni_1*log(y_Ni_1)+y_Ni_2*log(y_Ni_2));

L0_AlNi_Al=(-1)*14225-5.625*T;
L1_AlNi_Al=0;

L0_AlNi_Ni=(-1)*22050;
L1_AlNi_Ni=1115;

L0_Al_AlNi=L0_AlNi_Al;
L1_Al_AlNi=L1_AlNi_Al;

L0_Ni_AlNi=L0_AlNi_Ni;
L1_Ni_AlNi=L1_AlNi_Ni;

L_AlNi_Al=L0_AlNi_Al+L1_AlNi_Al*(y_Al_1-y_Ni_1);
L_AlNi_Ni=L0_AlNi_Ni+L1_AlNi_Ni*(y_Al_1-y_Ni_1);

L_Al_AlNi=L0_Al_AlNi+L1_Al_AlNi*(y_Al_2-y_Ni_2);
L_Ni_AlNi=L0_Ni_AlNi+L1_Ni_AlNi*(y_Al_2-y_Ni_2);

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G_xs=y_Al_1*y_Ni_1*(y_Al_2*L_AlNi_Al+y_Ni_2*L_AlNi_Ni)+...
    y_Al_2*y_Ni_2*(y_Al_1*L_Al_AlNi+y_Ni_1*L_Ni_AlNi);

G=G_ref+G_conf+G_xs;

G_dash=matlabFunction(diff(G,y_Al_1));
x=fsolve(G_dash,0.5);

% final answers
y_Al_1=x;
y_Al_2=(x_Al-a1*y_Al_1)/a2;
y_Ni_1=(1-y_Al_1);
y_Ni_2=(x_Ni-a1*y_Ni_1)/a2;

fprintf('The site fraction of Al in sublattice 1 : %d.\n',y_Al_1);
fprintf('The site fraction of Al in sublattice 2 : %d.\n',y_Al_2);
fprintf('The site fraction of Ni in sublattice 1 : %d.\n',y_Ni_1);
fprintf('The site fraction of Ni in sublattice 2 : %d.\n',y_Ni_2);

```

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.

*The site fraction of Al in sublattice 1 : 4.000000e-01.
The site fraction of Al in sublattice 2 : 4.000000e-01.
The site fraction of Ni in sublattice 1 : 6.000000e-01.
The site fraction of Ni in sublattice 2 : 6.000000e-01.*

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