Phase HW6

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1 Phase HW6 solutions

Geol 2460 HW6 11-14-16 @author: Eric Burdette

Solve and plot the regular solution equations for the Enstatite-Diopside solvus, spinodal points, and free energy of mixing vs composition given the phase diagram at ambient pressure:

```
In [1]: # first import neccesary modules
        import numpy as np
        from scipy.optimize import fsolve
        import matplotlib.pyplot as plt
        %matplotlib inline
```

1.1 Regular Solution Functions

Critical temperature from Phase diagram is ~1457C determined by interpolation. Define the regular solution functions below:

Mixing energy:

$$\Delta G^{reg} = RT\left((1 - X_{Di}) * ln(1 - X_{Di}) + (X_{Di}) * ln(X_{Di})\right) + \Omega(1 - X_{Di})X_{Di} \quad (1)$$

1st derivative:

$$\frac{d\Delta G^{reg}}{dX_{Di}} = 0 = RT\left(\frac{X_{Di}}{(1 - X_{Di})}\right) + \Omega(1 - 2X_{Di}) \quad (2)$$

2nd Derivative:

$$\frac{d^2\Delta G^{reg}}{dX_{Di}^2} = 0 = RT\left(\frac{1}{(X_{Di})} + \frac{1}{(1 - X_{Di})}\right) - 2\Omega 0 = X_{Di}^2 - X_{Di} + \frac{RT}{2\Omega} \quad (3)$$

```
In [2]: Tcrit=1457+273 #critical temperature from diagram is ~1457C
        Omega=2*8.314*Tcrit #regular solution parameter can be solved for and used

        Tlist=np.array([1450,1440,1425,1400,1300,1350,1200,1100,1000,800,600])+273


        def Gmix(Xb,T,omega): # regular solution delta G of mixing
            return 8.314*T*((1-Xb)*np.log(1-Xb)+Xb*np.log(Xb))+omega*Xb*(1-Xb)
```

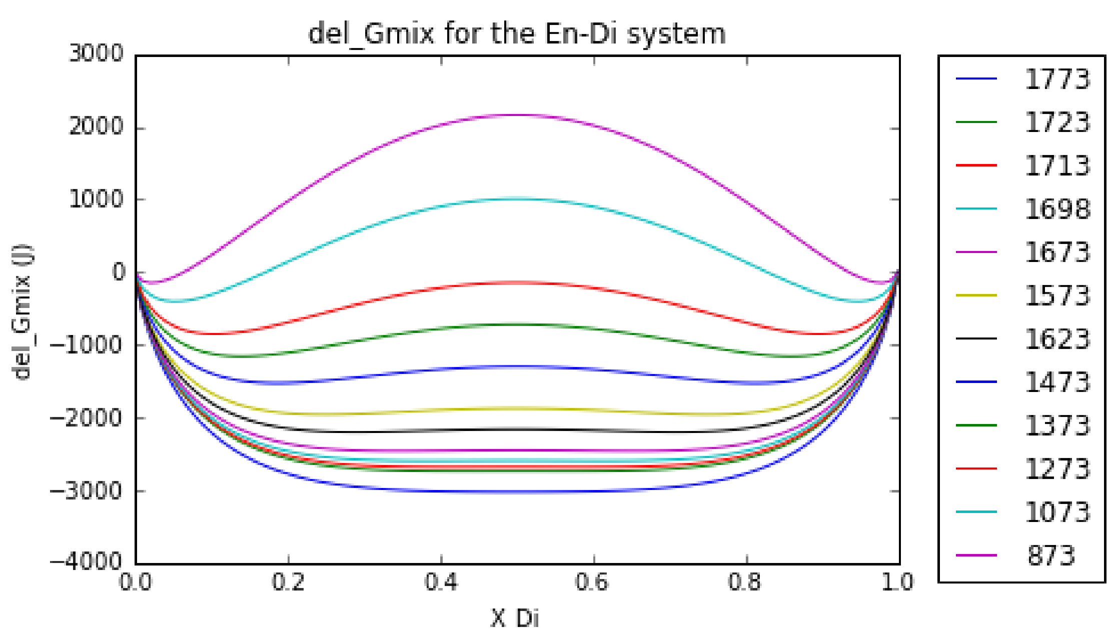
```
def spinodal(T,omega): # spinodal points are roots of second derivative
    if T<Tcrit:
        #polynomial is -R*T+2*omega*Xb-2*omega*x^2=0
        roots=np.roots([1,-1,8.314*T/(2*omega)])
        return roots[0],roots[1]
    else:
        return None

def Gmix_deriv(Xb,T,omega): # First derivative=0 close to either end-member
    return 8.314*T*np.log(Xb/(1-Xb))+omega*(1-2*Xb)
```

1.2 Mixing Free Energy Plot

Compute Equation (1) at specified temperatures (curves are in sequential order from lowest at 1773K to highest at 873K)

```
In [3]: #plot mixing free energies
        XbList=np.linspace(1e-5,1-1e-5,100)
        plt.plot(XbList,Gmix(XbList,1773,Omega), label='1773')
        for T in Tlist:
            GmixT=Gmix(XbList,T,Omega)
            plt.plot(XbList,GmixT, label=str(T))
        plt.legend(bbox_to_anchor=(1.05, 1), loc=2, borderaxespad=0.)
        plt.title('del_Gmix for the En-Di system'); plt.xlabel('X_Di'); plt.ylabel
        plt.show()
```



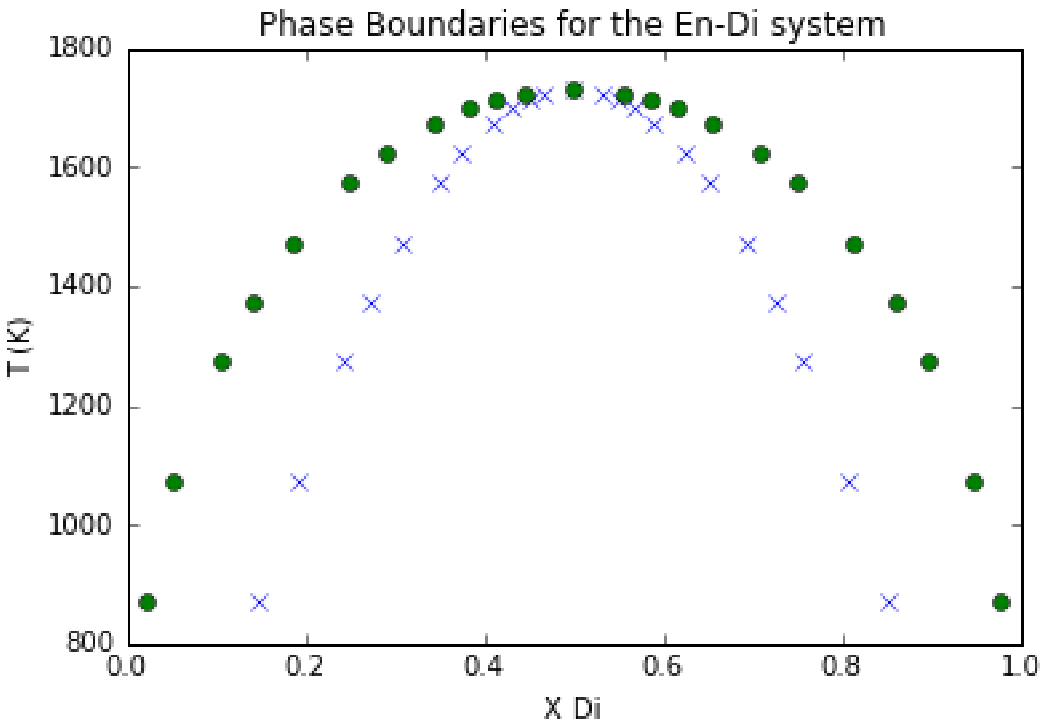
1.3 Spinodal/Solvus Calculations, Plot

Solve Equation (4) for the spinodal points
    Solve Equation (2) for minima nearest end members
    Print data and plot curves

In [4]:
```
#output solvus/spinodal points for a given temperature
Tspin=[]
xlist_spin=[]
xlist_solv=[]
print('T (K), left sovlus, left spinodal, right spinodal, right solvus')
for T in Tlist:
    sp2,sp1=spinodal(T,Omega)
    solv1=fsolve(Gmix_deriv,x0=0+1e-7,args=(T,Omega))[0] #numerically solve
    solv2=fsolve(Gmix_deriv,x0=1-1e-7,args=(T,Omega))[0] #'' for right solv
    Tspin.append(T);xlist_spin.append(sp1); xlist_solv.append(solv1)
    Tspin.append(T);xlist_spin.append(sp2); xlist_solv.append(solv2)
    print('{:04.0f}'.format(T),','+4*' ','{:01.4f}'.format(solv1),','+6*' '
Tspin.append(Tcrit);xlist_spin.append(0.5); xlist_solv.append(0.5)
```

```
T (K), left sovlus, left spinodal, right spinodal, right solvus
1723 ,     0.4450 ,       0.4682 ,        0.5318 ,       0.5550
1713 ,     0.4145 ,       0.4504 ,        0.5496 ,       0.5855
1698 ,     0.3831 ,       0.4320 ,        0.5680 ,       0.6169
1673 ,     0.3449 ,       0.4092 ,        0.5908 ,       0.6551
1573 ,     0.2487 ,       0.3494 ,        0.6506 ,       0.7513
1623 ,     0.2900 ,       0.3757 ,        0.6243 ,       0.7100
1473 ,     0.1866 ,       0.3073 ,        0.6927 ,       0.8134
1373 ,     0.1403 ,       0.2729 ,        0.7271 ,       0.8597
1273 ,     0.1042 ,       0.2430 ,        0.7570 ,       0.8958
1073 ,     0.0530 ,       0.1919 ,        0.8081 ,       0.9470
0873 ,     0.0221 ,       0.1481 ,        0.8519 ,       0.9779
```

In [5]:
```
#plot solvus/spinodal points
plt.plot(xlist_spin,Tspin,'x')
plt.plot(xlist_solv,Tspin, 'o')
plt.title('Phase Boundaries for the En-Di system'); plt.xlabel('X_Di'); plt
plt.show()
```


Phase Boundaries for the En-Di system
T (K)
X_Di
1800
1600
1400
1200
1000
800
0.0
0.2
0.4
0.6
0.8
1.0