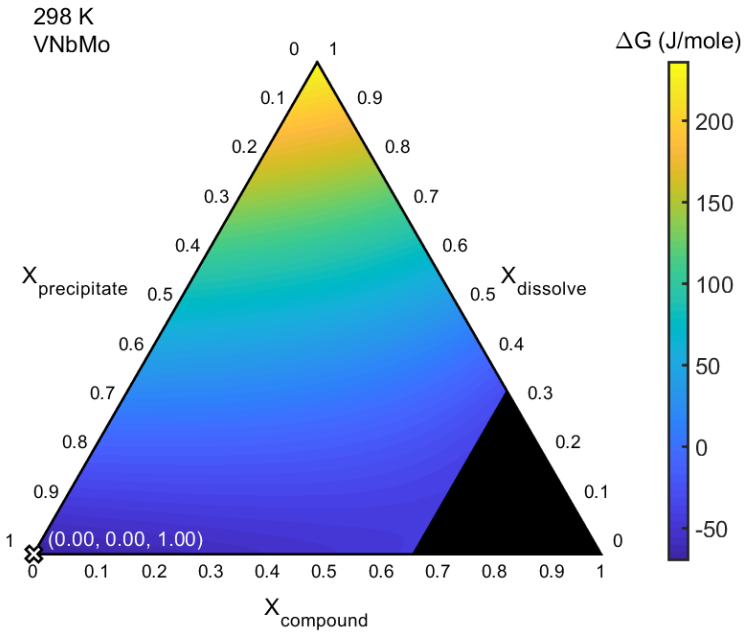
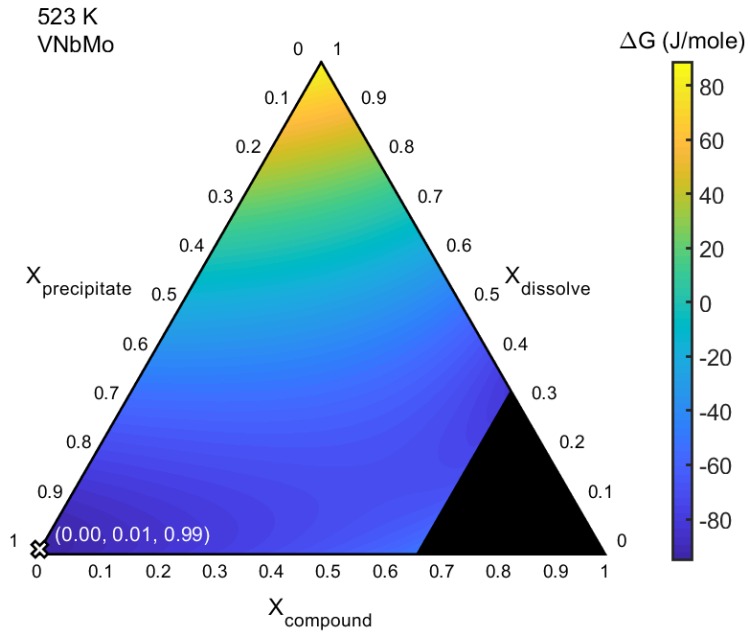
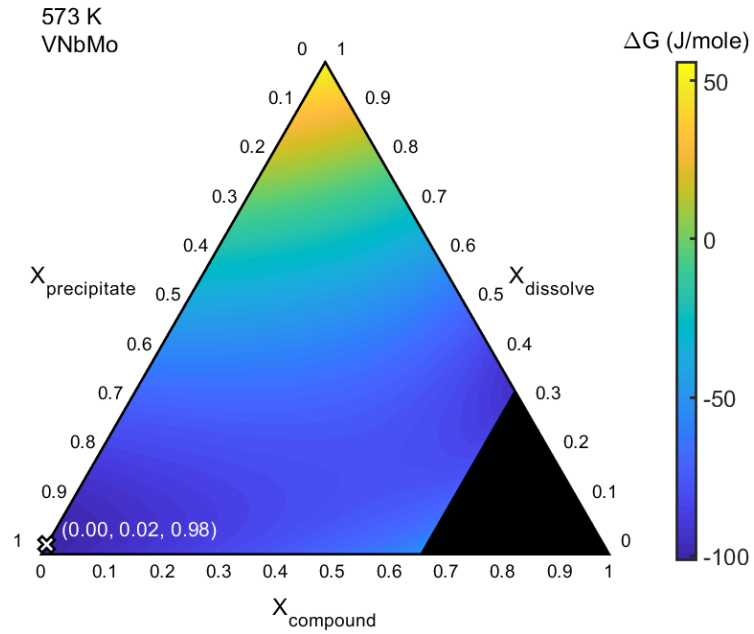
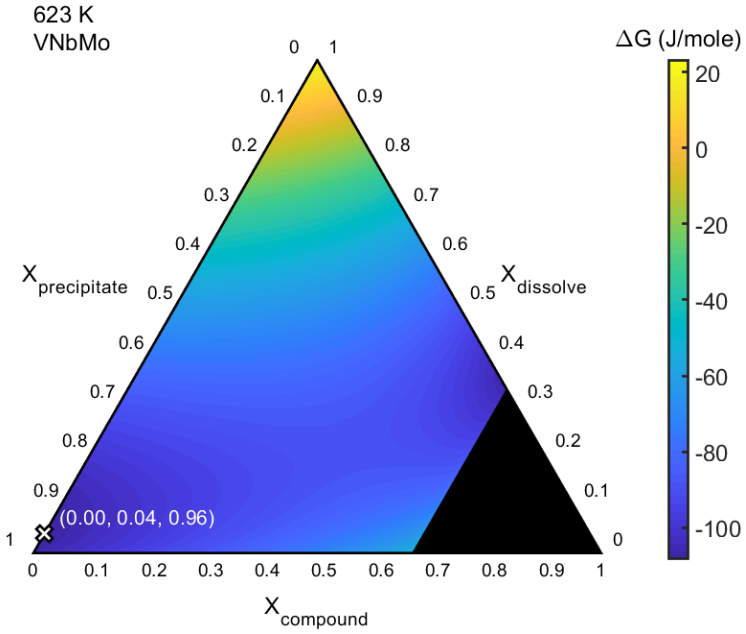
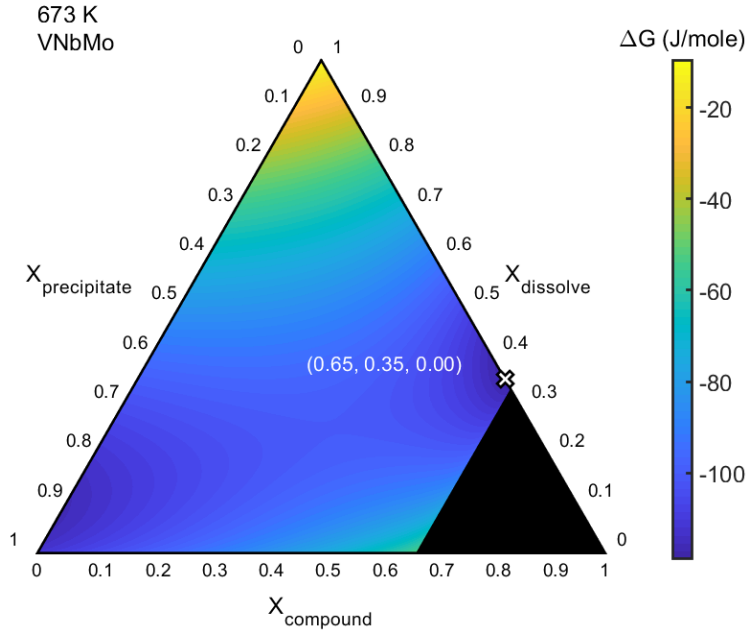










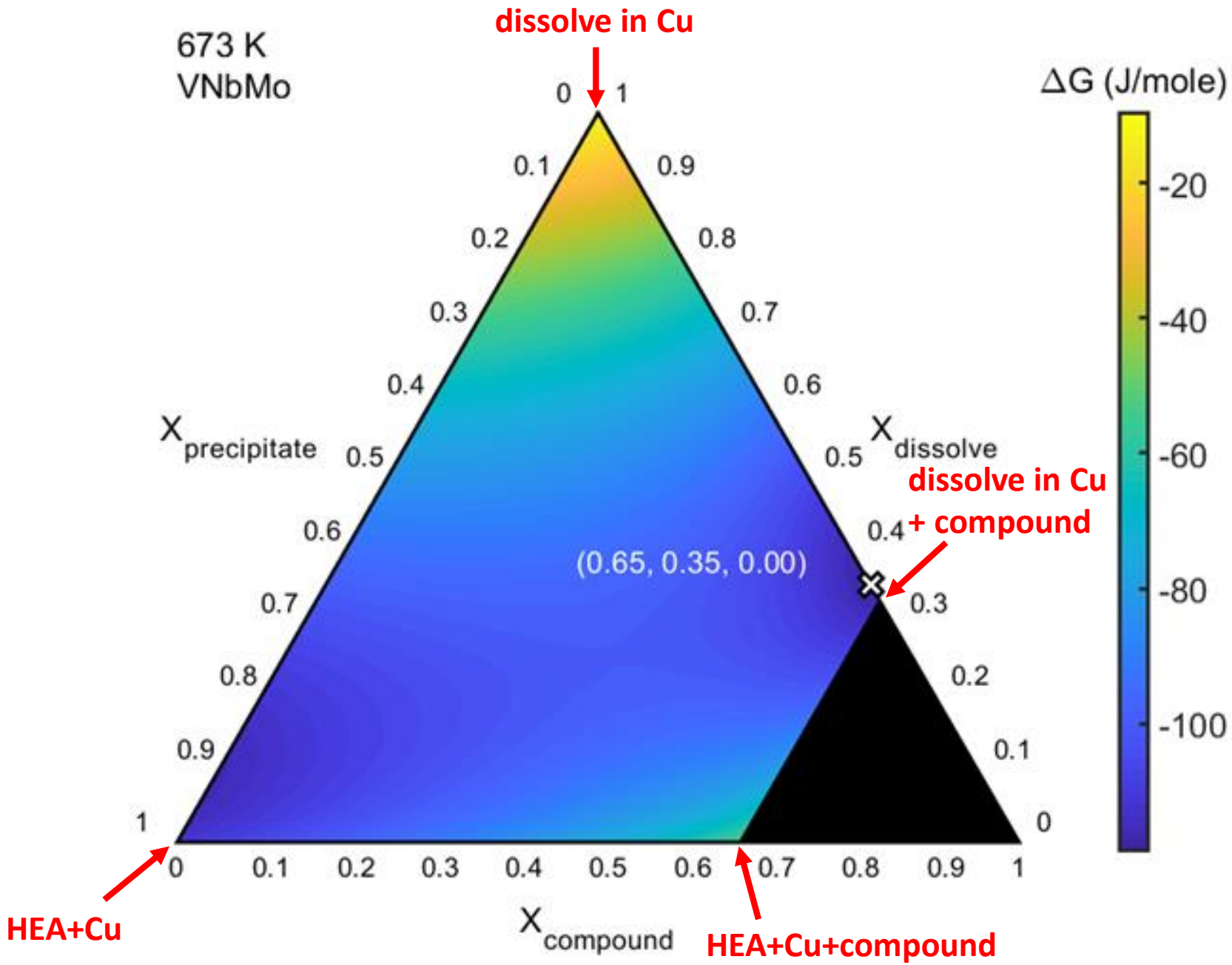
座標: $(X_{compound}, X_{dissolve}, X_{precipitate})$

$X_{compound}$ = 合金元素形成化合物比例

$X_{dissolve}$ = 合金元素固溶比例

$X_{precipitate}$ = 合金元素析出比例

e.g. 在673 K時，有65%的合金元素會形成化合物；剩下的合金元素固溶在Cu裡面，不形成析出相 (0.65, 0.35, 0.00)


673 K
VNbMo
dissolve in Cu
ΔG (J/mole)
-20
-40
-60
-80
-100
X precipitate
X dissolve
X compound
(0.65, 0.35, 0.00)
dissolve in Cu
+ compound
HEA+Cu
HEA+Cu+compound

```
clear
close all

TC = [25 250 300 350 400]; 溫度
for t = 1:5
    T = TC(t) + 273; % Temperature
    element = 'VNbMo'; 合金名稱
    fraction_compound = 0:0.01:1.01;
    fraction_dissolve = 0:0.01:1.01;
    for i = 1:length(fraction_compound)
        for j = 1:length(fraction_compound)-i+1
            %% input

            % --------------------------------------------------------
            % composition
            concentration = zeros(6,1);
            concentration(1) =  0.4; % V     合金成分(要改)
            concentration(2) =  0.4; % Nb
            concentration(3) =  0.4; % Mo   input concentration here!
            concentration(4) =    0; % Ta
            concentration(5) =    0; % W
            concentration(6) = 98.8; % Cu
            % --------------------------------------------------------

            X_c = fraction_compound(i); % compound fraction (0~1)
            X_ss = fraction_dissolve(j); % fraction of element not forming compound dissolve in Cu

            disp(['X_c = ',num2str(X_c)])
            disp(['X_ss = ',num2str(X_ss)])

```

```
% ------------------------------------------------------------
c_element(1) = 2;
c_element(2) = 3;
c_Stoichio(1) = 1; % e.g. Nb1Mo1, c_element(1) = 2 c_element(2) = 3
c_Stoichio(2) = 1; %              c_Stoichio(1) = 1 c_Stoichio(2) = 1;
% ------------------------------------------------------------

concentration_c = zeros(6,1);
concentration_c(c_element) = ...
    min(concentration(c_element)'./c_Stoich
    *X_c; % compound composition
concentration_ss = [(concentration(1:5) - c                    olid
concentration_p = concentration-concentrati


% thermodynamics

delta_H = zeros(6);
delta_H(:,1) = [0;-1;0;-1;-1;5];
delta_H(:,2) = [-1;0;-6;0;-8;3];
delta_H(:,3) = [0;-6;0;-5;0;19];
delta_H(:,4) = [-1;0;-5;0;-7;2];
delta_H(:,5) = [-1;-8;0;-7;0;22];
delta_H(:,6) = [5;3;19;2;22;0];

delta_H_c = [0.00, 0.00, 0.00, 0.00, 0.00;...
    0.00, 0.00, -9.40, 0.00, 0.00;...
    0.00, -9.40, 0.00,  -11.00, 0.00;...
    0.00, 0.00, -11.00, 0.00, -6.70;...
    0.00, 0.00, 0.00, -6.70, 0.00];
```

化合物種類/成分，如果是$NbMo_2$那就改成
c_element(1) = 2 (這是Nb)
c_element(2) = 3 (這是Mo)
c_Stoichio(1) = 1
c_Stoichio(1) = 2 (Nb/Mo反應計量1:2)