개인 과제물 (Mid-Term Report – 2022)

- Postechium (Ps)과 Tohokium(Tk) 2 원계에 대한 실험 정보는 다음과 같이 발표되어있다. 이를 바탕으로 Liquid, fcc, bcc 각 상에 대한 열역학 수식화를 수행하고 Ps-Tk 2 원계 상태도를 계산하시오.
  Calculate the phase diagram of the Ps-Tk binary system.

- Gibbs energy of pure Ps and Tk:

$$\Delta^o G_{Ps}^{fcc\rightarrow liquid} = 15000 - 12\ T$$

$$\Delta^o G_{Tk}^{bcc\rightarrow liquid} = 6000 - 10\ T$$

$$\Delta^o G_{Ps}^{fcc\rightarrow bcc} = 4000$$

$$\Delta^o G_{Tk}^{bcc\rightarrow fcc} = 7500$$

- Enthalpy of mixing (J/mol) in liquid

X_{Tk}	ΔH_m	X_{Tk}	ΔH_m
2.5E-02	3.60E+02	5.25E-01	3.087E+03
5.0E-02	6.96E+02	5.50E-01	3.034E+03
7.5E-02	1.008E+03	5.75E-01	2.966E+03
1.0E-01	1.297E+03	6.00E-01	2.884E+03
1.25E-01	1.564E+03	6.25E-01	2.789E+03
1.50E-01	1.807E+03	6.50E-01	2.679E+03
1.75E-01	2.029E+03	6.75E-01	2.557E+03
2.00E-01	2.230E+03	7.00E-01	2.423E+03
2.25E-01	2.409E+03	7.25E-01	2.276E+03
2.50E-01	2.568E+03	7.50E-01	2.118E+03
2.75E-01	2.707E+03	7.75E-01	1.949E+03
3.00E-01	2.826E+03	8.00E-01	1.769E+03
3.25E-01	2.926E+03	8.25E-01	1.579E+03
3.50E-01	3.007E+03	8.50E-01	1.379E+03
3.75E-01	3.070E+03	8.75E-01	1.170E+03
4.00E-01	3.115E+03	9.00E-01	9.522E+02
4.25E-01	3.142E+03	9.25E-01	7.256E+02
4.50E-01	3.153E+03	9.50E-01	4.911E+02
4.75E-01	3.147E+03	9.75E-01	2.491E+02
5.00E-01	3.125E+03		

- Activity of Tk in liquid at 1500 K (reference state: Liquid Tk)

X_{Tk}	a_{Tk}	X_{Tk}	a_{Tk}
2.50E-02	3.0619E-02	5.25E-01	5.0506E-01
5.00E-02	5.9569E-02	5.50E-01	5.2915E-01
7.50E-02	8.7099E-02	5.75E-01	5.5359E-01
1.00E-01	1.1342E-01	6.00E-01	5.7838E-01
1.25E-01	1.3875E-01	6.25E-01	6.0353E-01
1.50E-01	1.6323E-01	6.50E-01	6.2902E-01
1.75E-01	1.8704E-01	6.75E-01	6.5484E-01
2.00E-01	2.1031E-01	7.00E-01	6.8096E-01
2.25E-01	2.3316E-01	7.25E-01	7.0736E-01
2.50E-01	2.5570E-01	7.50E-01	7.3401E-01
2.75E-01	2.7802E-01	7.75E-01	7.6084E-01
3.00E-01	3.0023E-01	8.00E-01	7.8782E-01
3.25E-01	3.2239E-01	8.25E-01	8.1489E-01
3.50E-01	3.4458E-01	8.50E-01	8.4197E-01
3.75E-01	3.6686E-01	8.75E-01	8.6899E-01
4.00E-01	3.8929E-01	9.00E-01	8.9586E-01
4.25E-01	4.1191E-01	9.25E-01	9.2250E-01
4.50E-01	4.3476E-01	9.50E-01	9.4881E-01
4.75E-01	4.5788E-01	9.75E-01	9.7468E-01
5.00E-01	4.8131E-01		

● Enthalpy of Formation in FCC and BCC

in FCC		*in BCC*	
X_{Tk}	ΔH_f	X_{Tk}	ΔH_f
2.50E-02	4.902E+02	6.00E-01	3.280E+03
5.00E-02	9.564E+02	6.25E-01	3.140E+03
7.50E-02	1.399E+03	6.50E-01	2.993E+03
1.00E-01	1.819E+03	6.75E-01	2.835E+03
1.25E-01	2.217E+03	7.00E-01	2.670E+03
1.50E-01	2.593E+03	7.25E-01	2.496E+03
1.75E-01	2.949E+03	7.50E-01	2.313E+03
2.00E-01	3.285E+03	7.75E-01	2.121E+03
2.25E-01	3.602E+03	8.00E-01	1.920E+03
2.50E-01	3.900E+03	8.25E-01	1.710E+03
2.75E-01	4.179E+03	8.50E-01	1.493E+03
3.00E-01	4.442E+03	8.75E-01	1.266E+03
3.25E-01	4.688E+03	9.00E-01	1.030E+03
3.50E-01	4.918E+03	9.25E-01	7.856E+02
3.75E-01	5.132E+03	9.50E-01	5.325E+02
4.00E-01	5.332E+03	9.75E-01	2.706E+02
4.25E-01	5.518E+03		
4.50E-01	5.691E+03		
4.75E-01	5.851E+03		
5.00E-01	6.000E+03		

∴ Enthalpy of Formation 과 Enthalpy of Mixing 의 차이를 분명하게 고려할 것.

Distinguish the difference between the Enthalpy of Formation and Enthalpy of Mixing Clearly.

Activity of Ps in BCC and Activity of Tk in FCC at 600 K

in BCC (ref: FCC Ps)		*in FCC* (ref: BCC Tk)	
X_{Tk}	a_{Ps}	X_{Tk}	a_{Tk}
6.00E-01	1.24300E+00	2.50E-02	6.53900E-01
6.25E-01	1.19860E+00	5.00E-02	1.12090E-00
6.49E-01	1.15200E+00	7.50E-02	1.45418E-00
6.75E-01	1.10300E+00	1.00E-01	1.69170E-00
6.99E-01	1.05090E+00	1.25E-01	1.86084E-00
7.25E-01	9.95500E-01	1.50E-01	1.98140E-00
7.50E-01	9.36300E-01	1.74E-01	2.06000E-00
7.74E-01	8.72830E-01	2.00E-01	2.12990E-00
8.00E-01	8.04500E-01	2.24E-01	2.17595E-00
8.24E-01	7.30800E-01	2.50E-01	2.21140E-00
8.50E-01	6.51100E-01	2.75E-01	2.24040E-00
8.75E-01	5.64600E-01	3.00E-01	2.26600E-00
8.99E-01	4.70530E-01	3.24E-01	2.29060E-00
9.25E-01	3.68060E-01	3.49E-01	2.31580E-00
9.49E-01	2.56210E-01	3.75E-01	2.34300E-00
9.75E-01	1.33920E-01	4.00E-01	2.37310E-00
		4.25E-01	2.40696E-00
		4.49E-01	2.44507E-00
		4.74E-01	2.48790E+00
		5.00E-01	2.53582E+00

∴ 각 성분에 대해 활동도의 reference state 가 다르다는 것을 분명하게 고려할 것.

Consider that the reference state is different for individual elements

β 상에서,
reference state 가 α인 성분 i 의 Chemical potential 은 다음과 같이 두 가지로 나타낼 수 있다.
두 경우 활동도는 reference state 가 달라 값이 달라진다.

Activity values vary depending on the reference state chosen.

$$\mu_i^{\beta} = \Delta^o G_i^{\alpha \to \beta} + RT \ln a_i(wrt.\ \beta) = RT \ln a_i(wrt.\ \alpha)$$