개인 과제물 (학기 중간 평가용 - 2021)

- Postechium (Ps)과 Kaistium (Ks) 2 원계에 대한 실험 정보는 다음과 같이 발표되어있다. 이를 바탕으로 Liquid, fcc, bcc 각 상에 대한 열역학 수식화를 수행하고 Ps-Ks 2 원계 상태도를 계산하시오.

- 순수 Ps, Ks 의 Gibbs energy:

$$\Delta^o G_{Ps}^{fcc \rightarrow liquid} = 15000 - 10\ T$$

$$\Delta^o G_{Ks}^{bcc \rightarrow liquid} = 16250 - 12.5\ T$$

$$\Delta^o G_{Ps}^{fcc \rightarrow bcc} = 10000$$

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

- 액상에서의 Enthalpy of mixing (J/mol)

X_{Ks}	ΔH_m	X_{Ks}	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		

- 1500 K 액상에서 Ks 의 활동도 (reference state: Liquid Ks)

X_{Ks}	a_{Ks}	X_{Ks}	a_{Ks}
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_{Ks}	ΔH_f	X_{Ks}	ΔH_f
2.50E-02	4.902E+02	6.00E-01	5.679E+03
5.00E-02	9.564E+02	6.25E-01	5.390E+03
7.50E-02	1.399E+03	6.50E-01	5.092E+03
1.00E-01	1.819E+03	6.75E-01	4.785E+03
1.25E-01	2.217E+03	7.00E-01	4.469E+03
1.50E-01	2.593E+03	7.25E-01	4.145E+03
1.75E-01	2.949E+03	7.50E-01	3.812E+03
2.00E-01	3.285E+03	7.75E-01	3.470E+03
2.25E-01	3.602E+03	8.00E-01	3.119E+03
2.50E-01	3.900E+03	8.25E-01	2.760E+03
2.75E-01	4.179E+03	8.50E-01	2.392E+03
3.00E-01	4.442E+03	8.75E-01	2.015E+03
3.25E-01	4.688E+03	9.00E-01	1.629E+03
3.50E-01	4.918E+03	9.25E-01	1.235E+03
3.75E-01	5.132E+03	9.50E-01	8.324E+02
4.00E-01	5.332E+03	9.75E-01	4.206E+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.

- Activity of Ps in BCC and Activity of Ks in FCC at 1100 K

in BCC (ref: FCC Ps)		*in FCC* (ref: BCC Ks)	
X_{Ks}	a_{Ps}	X_{Ks}	a_{Ks}
6.00E-01	1.32237E+00	2.50E-02	1.14372E-01
6.25E-01	1.25056E+00	5.00E-02	2.13069E-01
6.49E-01	1.17781E+00	7.50E-02	2.99078E-01
6.75E-01	1.10403E+00	1.00E-01	3.74830E-01
6.99E-01	1.02911E+00	1.25E-01	4.42314E-01
7.25E-01	9.52960E-01	1.50E-01	5.03162E-01
7.50E-01	8.75457E-01	1.74E-01	5.58723E-01
7.74E-01	7.96497E-01	2.00E-01	6.10117E-01
8.00E-01	7.15967E-01	2.24E-01	6.58276E-01
8.24E-01	6.33748E-01	2.50E-01	7.03982E-01
8.50E-01	5.49717E-01	2.75E-01	7.47895E-01
8.75E-01	4.63748E-01	3.00E-01	7.90571E-01
8.99E-01	3.75708E-01	3.24E-01	8.32486E-01
9.25E-01	2.85460E-01	3.49E-01	8.74042E-01
9.49E-01	1.92859E-01	3.75E-01	9.15588E-01
9.75E-01	9.77581E-02	4.00E-01	9.57421E-01
		4.25E-01	9.99794E-01
		4.49E-01	1.04292E+00
		4.74E-01	1.08700E+00
		5.00E-01	1.13218E+00

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

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.

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