# 개인 과제물 (학기 중간 평가용 – 2)

- 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.

- 순수 Ps, Tk 의 Gibbs energy:

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

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

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

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

- 액상에서의 Enthalpy of mixing (J/mol)

| $X_{Tk}$ | $\Delta H_m$ | $X_{Tk}$ | $\Delta H_m$ |
|---|---|---|---|
| 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 Tk 의 활동도 (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* | |
|---|---|---|---|
| $X_{Tk}$ | $\Delta H_f$ | $X_{Tk}$ | $\Delta H_f$ |
| 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.

- 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.

**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.

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