Investigation of Gibbs free energy of bulk MoS_2 prepared through Spark Plasma Sintering technique

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Introduction

- Molybdenite (MoS_2) gray color mineral also a novel semiconductor with Indirect gap (E_G=1.3 eV) & High dielectric constant
- Interesting Mechanical, Optical & transport properties make MoS_2 an ideal candidate for Si substitute within (Opto)electronic technology
- High melting point (2500 K) make it difficult to fabricate MoS_2 in bulk morphology, Our sample Prepared using Spark Plasma Sintering (SPS) technique through controlling thermodynamical phase space journey

Method

- Combination of High P (90 MPa) **+** High Temperature (2100 K) being used in SPS technique to make 1" coin shape sample (See Pic →)
- Different characterization technique including SEM, PXRD, Hall, Optical Response, PIXE used to investigate the physical properties of fabricated sample
- Gibbs free energy (**G**) functionality of **T** & **P** calculated using related formula (see ↓) to understand thermodynamic phase space journey of MoS_2 during sintering process

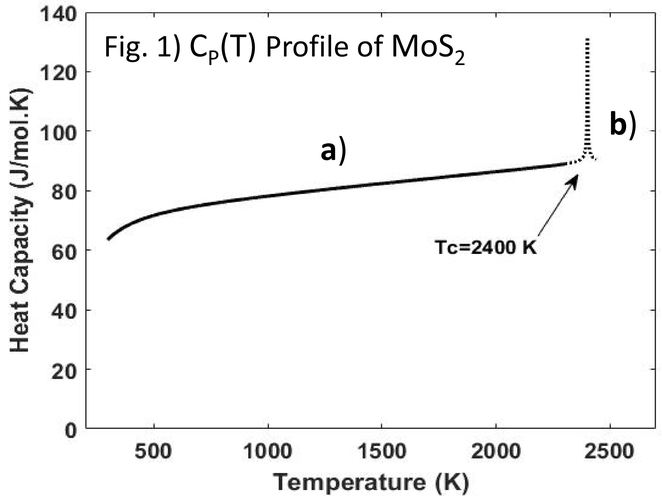
$$\Delta G = \Delta H - T\Delta S$$

$$\Delta H = H(P_2,T_2) - H(P_1,T_1)$$

$$= \int_{T_1}^{T_2} c_p dT + \int_{P_1}^{P_2} V(1-\alpha T)\, dP$$

$$\Delta S = S(P_2,T_2) - S(P_1,T_1)$$

$$= \int_{T_1}^{T_2} \frac{C_P}{T} dT - \int_{P_1}^{P_2} \alpha V dP$$



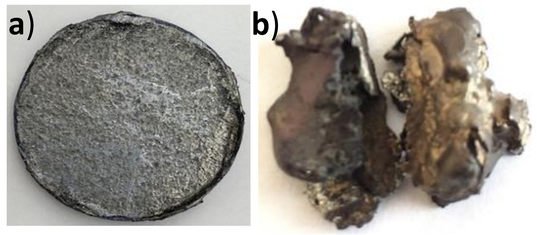


Fig. 2) Optical images of properly (**a**) & melted down (**b**) MoS_2 sintered samples

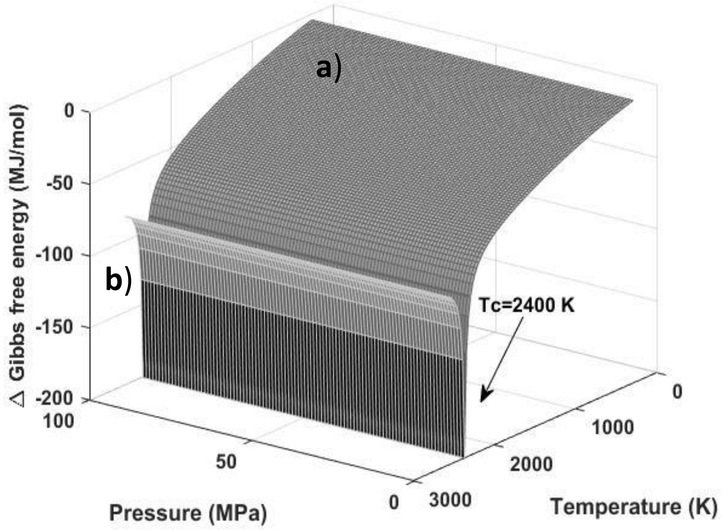


Fig. 3) G_{energy}(P,T) Profile of MoS_2 sample

Results

- Heat capacity profile $\mathbf{C_P(T)}$ of MoS_2 sample during SPS process calculated assuming melting as a structural 1st order phase transition @ $\mathbf{T_C}$**=2400** K (see Fig.1)
- Calculated Gibbs Free energy profile during sintering process as a function of **T** & **P** with at singularity behavior @ T_C (see Fig.3)

Discussion

- To make a Bulk polycrystalline MoS_2 sample using SPS technique, one need to have a control over how temperature profile being applied to powder sample That is why Gibbs free energy functionality calculated using semi-empirically method with related parameters

References

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