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Phase field modelling; The materials science, Mathematics and Computational aspects

Prof. M P Gururajan
Department of Metallurgical Engineering
And materials Science, IIT Bombay

Module No.1
Lecture No.1
Tutorial – 1

Welcome to this tutorial we are trying to see why in the case of condensed phases, you can assume that the internal energy and enthalpy or more or less the same. In other words the effect of pressure and volume changes need not be calculated at all, so this tutorial is based on introduction to thermodynamics of materials by Gaskell so, the addition that I have which is the fourth edition page number 134 to 136 this is described and that is what we are going to follow. So the idea is as follows so let us say that I take a system from state of (P_1 T),

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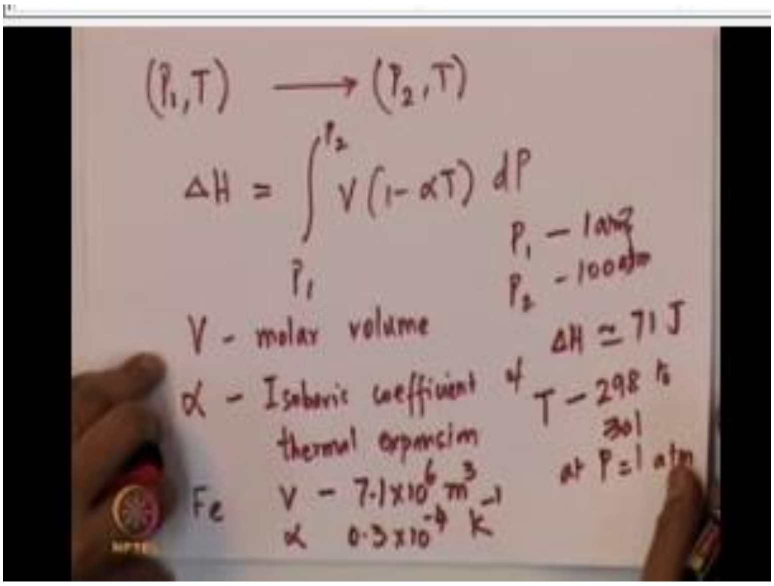

$(P_1, T) \longrightarrow (P_2, T)$

$$\Delta H = \int_{P_1}^{P_2} V(1-\alpha T)\, dP$$

V - molar volume

α - Isobaric coefficient of thermal expansion

Fe $V - 7.1\times10^{-6}\ m^3\ mol^{-1}$

$\alpha\ 0.3\times10^{-4}\ K^{-1}$

P_1 - 1atm

P_2 - 100atm

$\Delta H \simeq 71\ J$

T - 298 to 301 at P = 1 atm

So to state (P_2 T) now I want to calculate what is the change in enthalpy associated with this change going from p1 to p2? Let me call that change as $\Delta H = \int_{p1}^{p2}$ V times 1 -α T DP where V is the molar volume, and α is the isobaric coefficient of thermal expansion. Now if you take the example of iron for example suppose if I say I am considering iron F_e - 7.1 $\times 10^{6}$ m^3, this is the molar volume and α 0.3× 10-^{4} K^{-1}.

So if you use these two values and if you see that suppose if P1 is 1 atmospheric pressure, and P2 is 100 atmospheric pressure, you can calculate this quantity and you can show that Δ H = 71j, but this is for changing from one 200 atmosphere pressure.

On the other hand you can achieve the same 71 j change in the enthalpy by changing the temperature, if temperature changes from T 298 to 301 at P = 1atm you will get the same change in enthalpy, in similar fashion of course.

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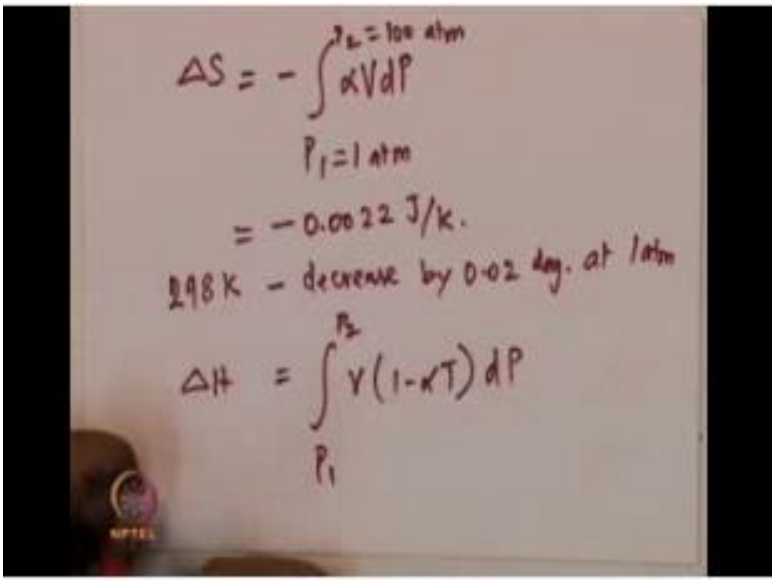

$$\Delta S = -\int_{P_1 = 1\,\text{atm}}^{P_2 = 100\,\text{atm}} \alpha V dP$$

$$= -0.0022\ \text{J/K}.$$

298K - decrease by 0.02 deg. at 1atm

$$\Delta H = \int_{P_1}^{P_2} V(1-\alpha T)\,dP$$

Of course you can also calculate the change in entropy and that is given by, again for a change of P_1 to 100 atm, So that is going to be of the order of -0.0022 J/k, and this change in entropy for example can be achieved in iron from 298 Kelvin suppose if you reduce the temperature decrease the temperature by 0.02deg, okay at 1atm, in other words the changes that are associated with pressure and volume and the in the entropy and enthalpy or very small in fact smaller temperature changes will cause much greater change in entropy and enthalpy.

Of course because these two are integral so on the $\Delta H = \int_{p1}^{p2} v\ (1 - \alpha\ T)\ d\ P$, it is possible that the molar volume and the α, the isobaric coefficient of thermal expansion or pressure dependent so they can be made functions of pressure and similarly here α P Vp dP, so it could be some polynomial that you are trying to integrate.

Again if you are going to be looking at very small changes in pressure, and typical changes that we have been talking about is between zero atmospheric pressure, and one atmospheric pressure so in that range this change in αRV with pressure is also very negligible, and unless you are going to have very large changes in pressure you know of the order of 100 atmospheric pressure change, but even that is going to produce changes in enthalpy and entropy which are achieved by fraction of a degree to a few degrees. So this is the reason why in condensed systems, that is liquids and solids we all assume we make this approximation.

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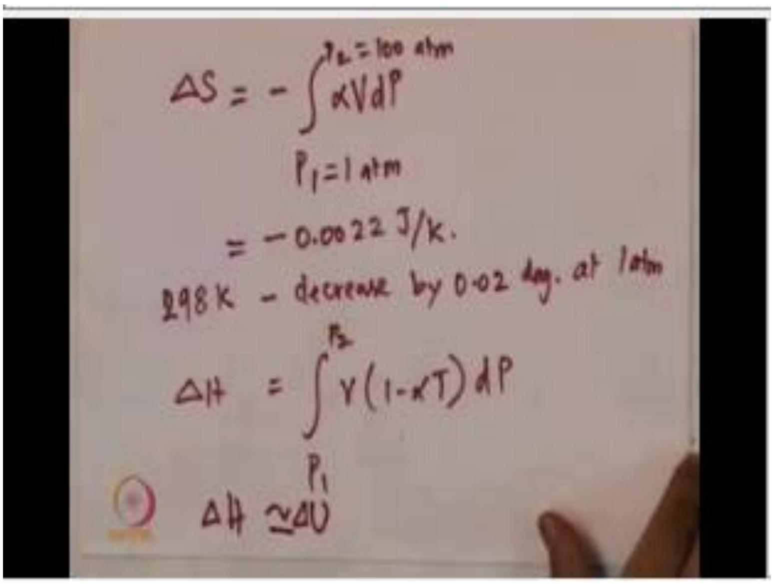

$$\Delta S = -\int_{P_1 = 1\,\text{atm}}^{P_2 = 100\,\text{atm}} \alpha V \, dP$$

$$= -0.0022\ \text{J/K}.$$

298K - decrease by 0.02 deg. at 1atm

$$\Delta H = \int_{P_1}^{P_2} V(1 - \alpha T)\, dP$$

$$\Delta H \simeq \Delta U$$

That is a Δ H = Δ U, so this is one of the approximations that we have made and this is a valid approximation for this reason, we have taken the example of iron you can take any other example it does not even have to be a solid you can even take the case of a liquid, molar volume changes are not very much and, expansion coefficients are not large numbers so because of which we always find that this approximation is a very good approximation thank you.

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IIT Bombay

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