Dynamic Behaviour of Materials

Prof. Prasenjit Khanikar
Department of Mechanical Engineering
Indian Institute of Technology-Guwahati

Lecture-22
Equations of States (Shock Waves) Theoretical Calculations

Hello everyone, so we have discussed about the experimental methods to obtain the EOS equation of state of shock waves. So in this lecture we will discuss about the theoretical calculations of obtaining the EOS the equation of state.

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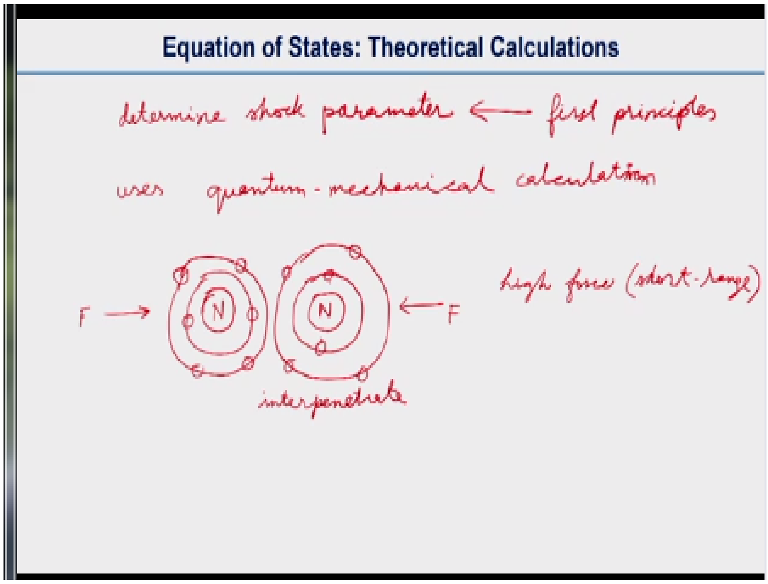

Equation of States: Theoretical Calculations

determine shock parameter ← first principles

uses quantum-mechanical calculation

So the theoretical calculations we can determine the shock parameters, shock parameters from first principles. You know that the first principles are the first basis are like propositions or assumptions those cannot be deduced from other principles. So and also it is possible calculate this in few cases the equation of state and for this theoretical calculations it is calculation uses quantum mechanical calculations that you know the quantum mechanics that involves the consideration of subatomic the structure.

So let us imagine a group of atoms compressed together let us say we will draw only 2 atoms here. So this is a nucleus and we have electron shells around it, so this n is the nucleus and then we have electrons here, we have electrons on the electron shells and then we will draw one more atom with nucleus here and these electrons shells here. So these are electrons this is just a representative image.

So if we compress it let say the group of atoms we are here we are drawing only 2 of them. So if we compress them we know these electron shells will interpenetrate and there will be very high force in between these atoms, so high forces and these are high forces when you compress it high forces regenerate and but they are short range for it involves only that inter-atomic distances short range.

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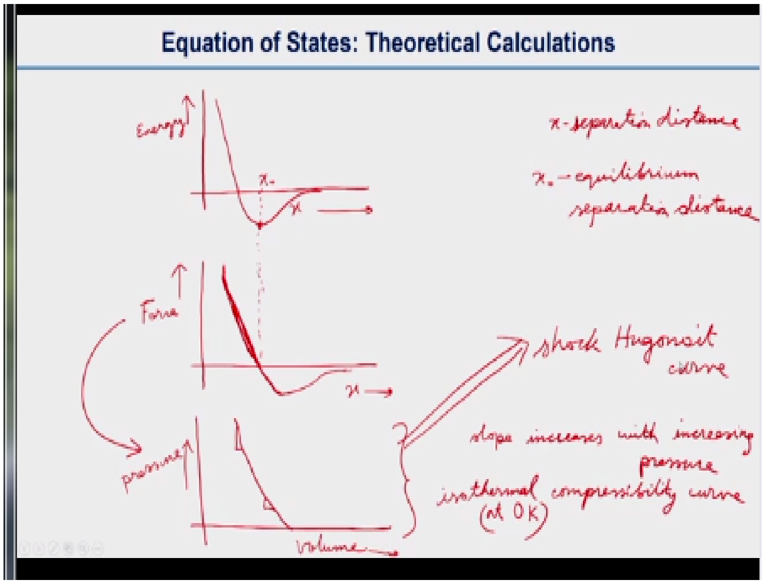

Equation of States: Theoretical Calculations

x - separation distance

x_0 - equilibrium separation distance

shock Hugonoit curve

slope increases with increasing pressure

isothermal compressibility curve (at 0 K)

So we have you studied this in during your engineering or even earlier classes that we can draw this energy versus separation distance diagram for these inter atomic interactions that we know energy versus x which is your x is our inter atomic distance or we can write separation distance. So this curve you most of you know that, so it looks like something like this and then from that we can even have force versus inter-atomic distances.

So this is the point of minimum energy, so this point that this separation distance let us say we say x0, the x0 is the equilibrium separation distance. So that term will be at equilibrium if they are separated by that much distance and then for force we know that we take it here the force will be 0 that it will look something like this. Because if we have higher inter-atomic distances than this separation distance.

Then it will have attractive forces here attractive forces and if you go below the inter-atomic that equilibrium separation distance it will have a repulsive forces. So that means when you were compressing the material it will have repulsive forces and we decrease in separation distance the inter-atomic forces will increase and that will increase to very high level. So I think we should have a it like a different slope not like this.

So slope will so and then again from this force separation distance that plot we can get pressure versus volume plot. So this will look like something like this, so this slope will be higher here and this slope will be lower here. So that means the increases slope increases with increasing pressure, so this is called this diagram is called isothermal compressibility curve that is actually isothermal that is at 0 Kelvin and so as I mention.

So this pressure volume curve can be obtained from this force separation distance curve. So these PV curve, so that means the pressure volume curve can also be used to obtained a shock Hugonoit curve.

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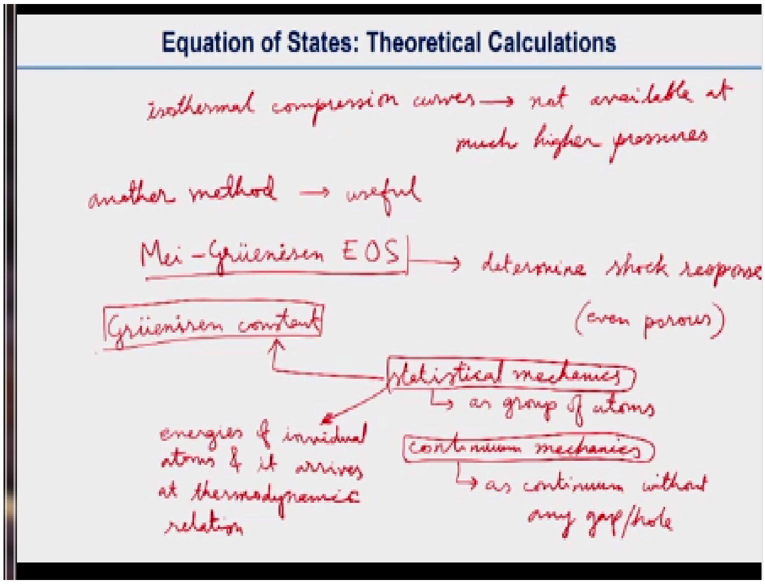

Equation of States: Theoretical Calculations

isothermal compression curves → not available at much higher pressures

another method → useful

Mei-Grüenisen EOS → determine shock response (even porous)

Grüenisen constant ← statistical mechanics

statistical mechanics → energies of invidual atoms & it arrives at thermodynamic relation

statistical mechanics ↳ as group of atoms

continuum mechanics ↳ as continuum without any gap/hole

So earlier researcher and then the early researchers they obtained shock compression curve for large number of materials by applying a high pressure but these isothermal curves. So those isothermal compression whatever we show just now isothermal compression curves, curves are not available at higher pressures at you can see the much higher pressures like in pressure greater than 10 Giga Pascal also.

So there is another method that is why which is more useful another method useful is called Mie-Gruneisen method it is pronounce as Mei I think Gruneisen, so this 2 dots for difference in pronunciation for this I think this german word. So this is called Mei-Gruneisen EOS, so this is another theoretical calculation, so this is important to this EOS is important to determined the shock and shock response of the materials or specially we can also do it even for the porous materials.

So this that the constant involved in this equation of straight that is Gruneisen constant. So that can be that constant can be obtained from statistical mechanics, so statistical mechanics as some of you know as oppose to continuum mechanics, so continuum mechanics is another one. So continuum mechanics I mean consider the material as continuum without any gap or hole.

But in statistical mechanics it treats as the material is group of atoms and actually the statistical mechanics it deals with the energies of individual atoms and it can be it arrives at thermodynamic relations that mean that can be related to the energies of the individual atoms can be related to the thermodynamic relations like thermodynamic relations that you know so that can be connected.

So note that as you can understand the continuum mechanics is different that and statistical mechanics are different. So to get the constant used in Mei-Gruneisen EOS equation of state that is the Gruneisen constant, so what we need to use some theories from statistical mechanics.

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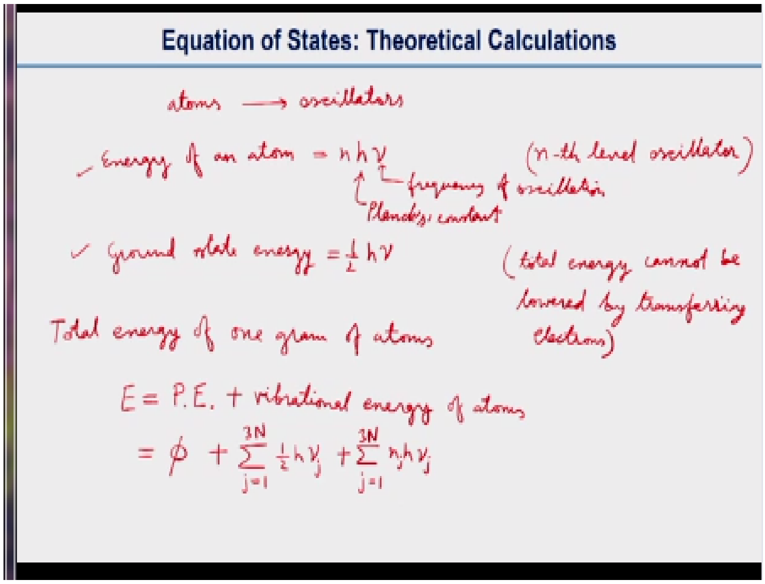

Equation of States: Theoretical Calculations

atoms → oscillators

✓ Energy of an atom $= n h \nu$ (n-th level oscillator)

frequency of oscillation

Planck's constant

✓ ground state energy $= \frac{1}{2} h \nu$

(total energy cannot be lowered by transferring electrons)

Total energy of one gram of atoms

$$E = P.E. + \text{vibrational energy of atoms}$$

$$= \phi + \sum_{j=1}^{3N} \frac{1}{2} h \nu_j + \sum_{j=1}^{3N} n_j h \nu_j$$

In this treatment this atoms are assumed as oscillators because of the atomic vibration we discussed in one of the first classes about the atomic vibrations, so atoms are assumed as oscillators. So energy of an atom due to this oscillation is nh mu, so it is called nth level oscillator and so this is Planck's constant and then this is the frequency of vibration or oscillation of those atoms.

So also there is one state called ground state that ground state energy is half h mu, so which is not included in that this energy and this is different. So ground state means that the total energy of the electrons cannot be lowered at that state total energy cannot be lowered by transferring electrons. So the total energy of an atom or let us assume a group of atom that means 1 gram let us say of atoms one gram of atoms of a material .

Now we can write E equal to the potential energy I will write PE for potential energy and then the vibrational energy**,** so of the atoms. So now the potential energy we can write it as C and then vibrational energy includes both the ground state and then the higher level state and nth level. So what we can do is we have now 1 gram of atoms, so there are not only single atom.

So we will write the summation from ij = 1 to 3 N I hope you know about this summation science. So this h, h is the Planck's constant will be constant and the frequency of vibration it will take for different atoms, so then j = 1 to (()) (16:18) N h mu j nj.

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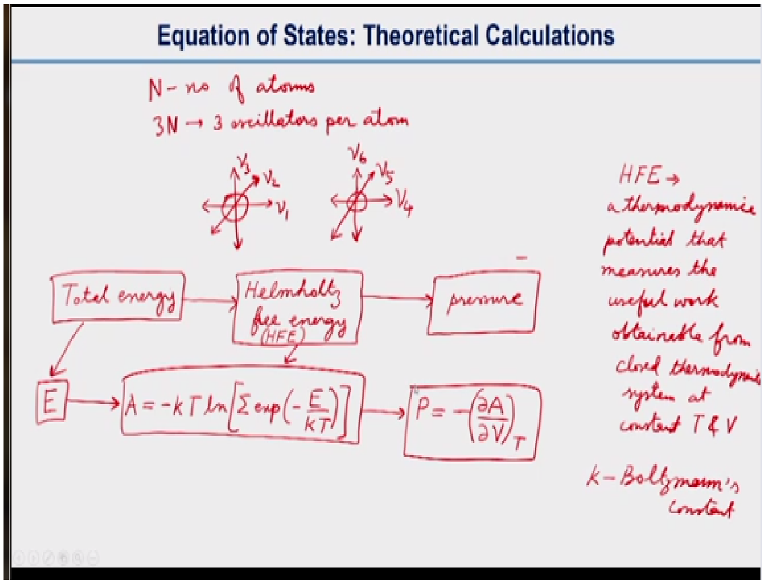

Equation of States: Theoretical Calculations

N - no of atoms

3N → 3 oscillators per atom

$A = -kT \ln\left[\sum \exp\left(-\frac{E}{kT}\right)\right]$

$P = -\left(\frac{\partial A}{\partial V}\right)_T$

HFE → a thermodynamic potential that measures the useful work obtainable from closed thermodynamic system at constant T & V

k - Boltzmann's constant

So here why we are writing 3N because we have N number of atoms and 3N because 3 oscillators, oscillators per atom which means in 3 oscillations in 3 directions. So if you see if you assume one atom here then oscillations are like this direction perpendicular direction and the perpendicular to these 2 directions will be we can write it like this. And then this will be let us say the frequency here the this oscillation frequency mu 2 and this will be again 3.

So similarly you have that we will have other atoms other just an atom will have similarly so you will have these frequencies 3 sorry. We can write let say 4, 5, 6, so similarly you can get you know thousands of atoms probably in this group of atoms or thousands or even more than that. So now that is why we understood that we use 3N as 1 atom can be considered as 3 oscillators the total energy we can use this total energy to find the thermodynamic potential Helmholtz free energy.

And then these Helmholtz free energy can be use to get the pressure, we are discussing about shock waves, so we want to know the pressure. So this Helmholtz free energy is a thermodynamic potential, this Helmholtz free energy we can write let say we can write it like HFE just have revision we are using. So this HFE is a thermodynamic this is a thermodynamic potential that measures the useful work obtainable from a closed thermodynamics system at constant temperature and volume.

So I will not derive these equations we just need to we want to just summarize it, so we will just write the expression we are not going to derive it do not worry about the derivations. And if you are interested you can go through the Mark Meyers the book of dynamic behavior materials which we referred as a the textbook that is in the chapter number 5 the shock waves equation of states.

So this is the total energy E, so from total energy E what we got is the almost free energy E and A = - kT. So k is the Boltzmann constant - kT (()) (21:15) summation of it is a exponential - E kT that E there is a total energy what we found and this is the expression for this is the total energy we talked about and this is almost free energy and then we will have the expression for pressure from Helmholtz free energy which is minus partial of A with respect to V then this will be at constant temperature.

So differential of HFE which respect to volume at constant temperature will give us the pressure and this pressure I will just write the final expression without going into the derivation.

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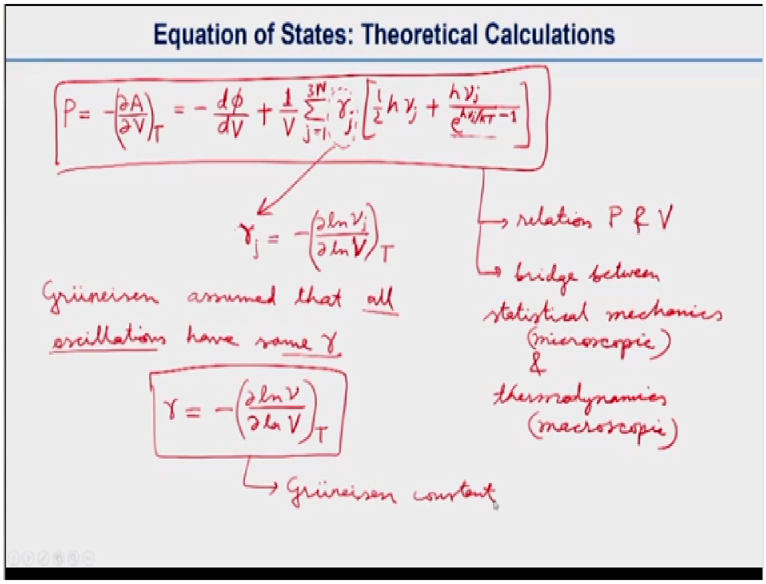

Equation of States: Theoretical Calculations

$$\boxed{P = -\left(\frac{\partial A}{\partial V}\right)_T = -\frac{d\phi}{dV} + \frac{1}{V}\sum_{j=1}^{3N} \gamma_j \left[\frac{1}{2}h\nu_j + \frac{h\nu_j}{e^{h\nu_j/kT}-1}\right]}$$

$$\gamma_j = -\left(\frac{\partial \ln \nu_j}{\partial \ln V}\right)_T$$

→ relation P & V

→ bridge between statistical mechanics (microscopic) & thermodynamics (macroscopic)

Grüneisen assumed that all oscillation have same γ

$$\boxed{\gamma = -\left(\frac{\partial \ln \nu}{\partial \ln V}\right)_T}$$

→ Grüneisen constant

It will be a, it is a long derivation because it needs some statistical mechanics input here, so this expression will look like something like this because it involves the total energy 3N gamma j. I will tell you what is gamma j and then half of h mu j + h mu j e to the h mu j kT - 1 this is e to the power this and that. So these terms it came from the statistical mechanics consideration we are not going to that but we are more interested in this parameter gamma j.

So gamma j is minus partial of ln mu j partial of ln V, so V is the volume and mu j is the as you know that frequency of vibration at constant temperature ok, so this is the gamma j. And this relation, if you see this relation that is a, you can tell that this is a relation between pressure and volume that you can see and also it is a bridge between statistical mechanics and thermodynamics.

As you know when you say thermodynamics it is basically we are talking about the macroscopic level and in statistical mechanics we are talking about microscopic level. So why I said that this is the bridge because the what we got it here is a relation between pressure and volume that is like thermodynamics and from where we got though we use there some relations of statistical mechanics.

As I told these terms came from statistical mechanics although we did not show the entire derivations, so that is why this is a bridge between statistical mechanics and thermodynamics and so Gruneisen simplified this and assume that all the oscillations have same gamma. So what it says is that gamma = - ln V T, we do not have a gamma J here or gamma j here or gamma subscript j or that mu subscript j.

So it says that all oscillations have the same gamma, so that is the assumption to make it the simplified, so this gamma as Grunei assume this and that this is called Grunei constant**,** so Gruneisen constant will be required.

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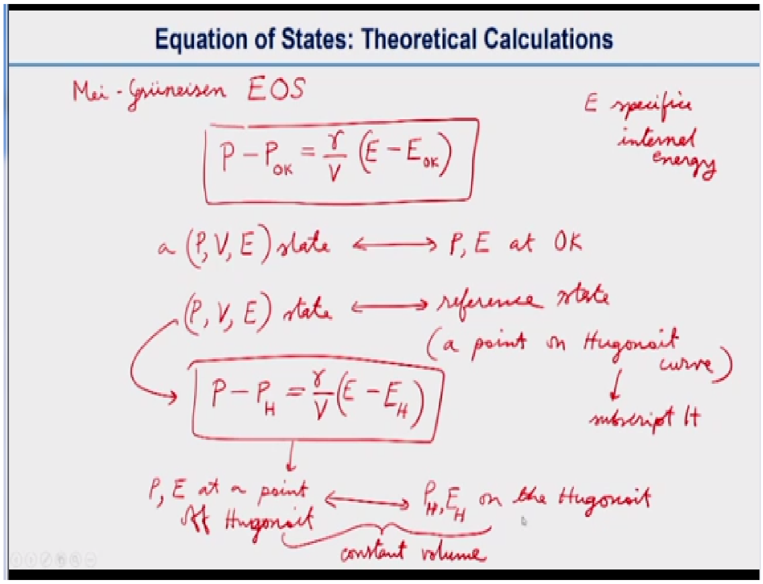

Equation of States: Theoretical Calculations

Mei-Grüneisen EOS

$$\boxed{P - P_{0K} = \frac{\gamma}{V}\left(E - E_{0K}\right)}$$

E specific internal energy

a (P, V, E) state ⟷ P, E at 0K

(P, V, E) state ⟷ reference state (a point on Hugoniot curve)

↓ subscript H

$$\boxed{P - P_H = \frac{\gamma}{V}\left(E - E_H\right)}$$

P, E at a point off Hugoniot ⟷ P_H, E_H on the Hugoniot

constant volume

Because we will write now the Mei Grunei equation of state, Grunei so that is what we were showing that is a theoretical calculation of shock wave. So we are not deriving these equations, we just will write the expression this is pressure at 0 Kelvin and then gamma V, E which is specific internal energy - E at 0 Kelvin. So this is at 0 Kelvin, so as you know E is the specific internal energy.

So this is Mie-Grunei equation of state, so what it they relates is a state thermodynamic state of P, V, E state it relates to P E at 0 Kelvin temperature. And it can also relate we can do this P V state to relate to any other reference state, for example what we can do is we can take a point on the Hugoniot curve. So that means then we can write P - P H = gamma V, V is the volume E - epsilon H subscript H.

So the subscript H means Hugoniot curve, a point on a Hugoniot curve is that subscript H, so this means that we show this equation but this means the pressure and specific internal energy at a point of Hugoniot that is outside Hugoniot curve of Hugoniot to this relate to a point P and E on the Hugoniot curve. So that means we wrote it as P subscript h and E subscript h.

So this happening at constant volume, so at constant volume so we can relate the pressure and internal specific as for a specific internal energy at a half Hugoniot point to a point on the Hugoniot.

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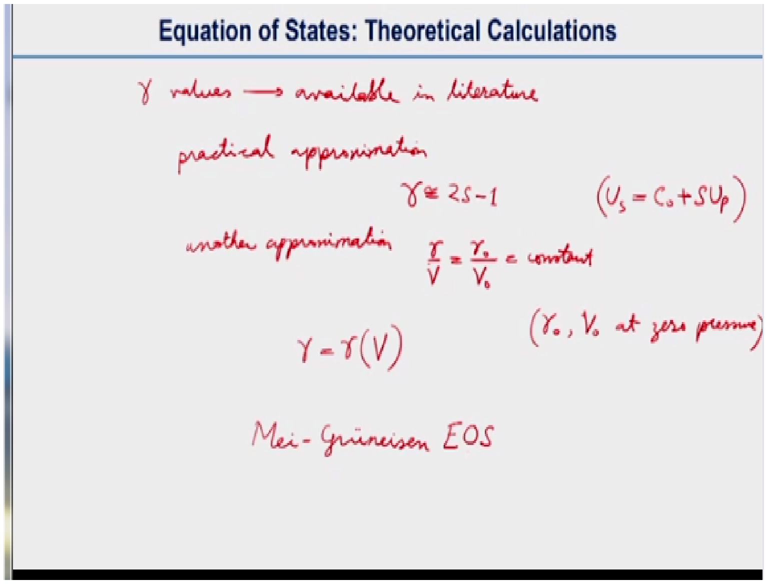

Equation of States: Theoretical Calculations

γ values → available in literature

practical approximation

$\gamma \cong 2s-1$ $(U_s = C_0 + SU_p)$

another approximation $\frac{\gamma}{V} = \frac{\gamma_0}{V_0} = \text{constant}$

$\gamma = \gamma(V)$ (γ_0, V_0 at zero pressure)

Mei-Grüneisen EOS

And this Grunei constant values for many materials are available in literature not for all the materials that we know that but for many materials it is available. And if you want to approximate a practical approximation is gamma = twice s - 1 you can write this is approximation, so twice s you know what is as this is comes from the linear the equation of state we know that C0 + s U p.

So that s you are using and this is twice as one that is a approximation you can assume and then another approximation is that gamma V = gamma naught V0 equal to constant, so these are at 0 pressure actually gamma0 V0 = constant, so these are at 0 pressure actually gamma0 V0 at 0 pressure. So this can be also sometimes useful and this gamma is actually assumed to be a function of volume. So this is for what we talked about for Mie-Gruneisen equation of state.

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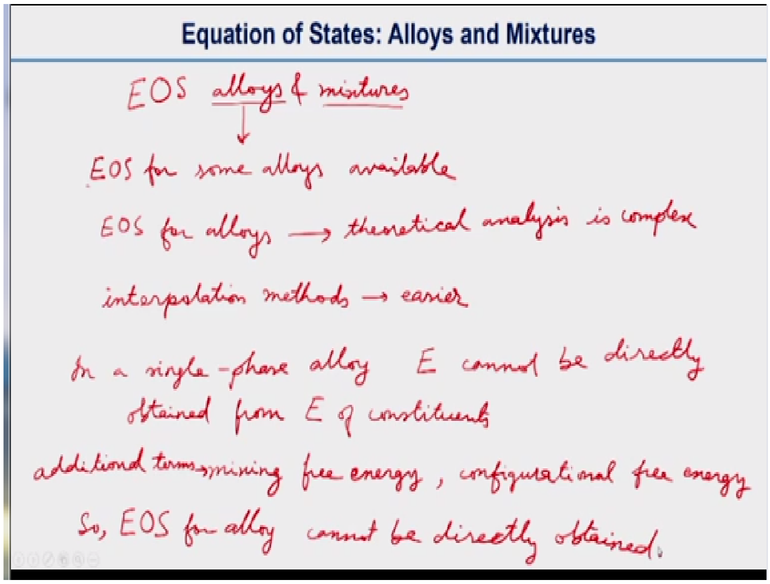

Equation of States: Alloys and Mixtures

EOS alloys & mixtures

↓

EOS for some alloys available

EOS for alloys → theoretical analysis is complex

interpolation methods → easier

In a single-phase alloy E cannot be directly obtained from E of constituents

additional terms, mixing free energy, configurational free energy

So, EOS for alloy cannot be directly obtained.

So we will now talk about equation of states for alloys and mixtures, so before going to that we need to know what is the difference between alloys and mixtures. So I will leave that part to you, so please study that what is the difference of alloys and mixtures, so the basic difference is the alloys have so nicely mix that it has a homogenous composition. So mixtures have separable structures but the for details you just please study about alloys and mixtures that is important.

So alloys for EOS equation of state for alloy is not very easy although it is easier for mixtures. So we know that for many alloys the equation of state is already available let us say we write at some alloys are EOS for some alloys available in the literature for some unknown material if we want to know for some unknown alloy, so you need to find the equation of state that we need to theoretically calculate EOS for alloys is not very easy.

So the theoretical analysis is complex, so we will here we will try some interpolation methods which are easier for an alloy let us say in a single phase alloy. So it is the specific internal energy that E cannot be directly obtained from the constituent of E the constituents why because there are other terms involved here, so these are like mixing free energy configurational free energy.

So these are additional terms, energy terms is required, so that is why so EOS for alloy is a alloy cannot be directly obtained here what we can do as I we mentioned that we use some interpolation method.

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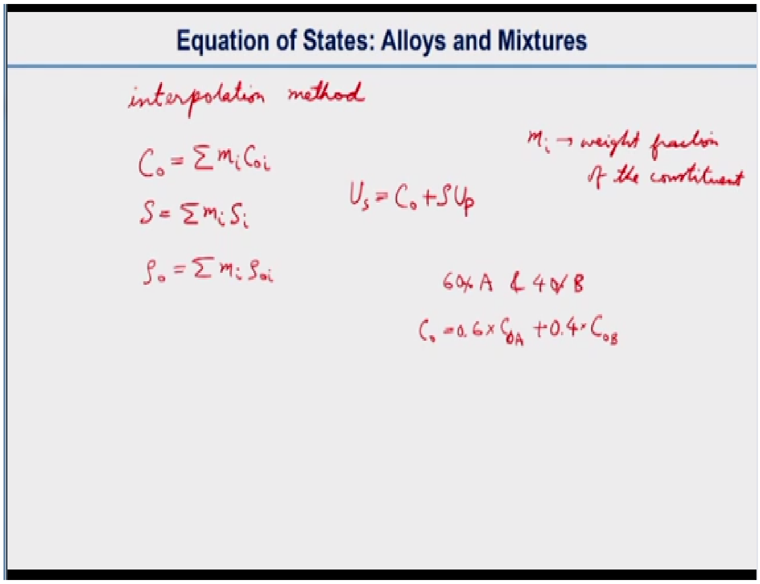

Equation of States: Alloys and Mixtures

interpolation method

$C_0 = \sum m_i C_{0i}$

$S = \sum m_i S_i$

$\rho_0 = \sum m_i \rho_{0i}$

$U_s = C_0 + S U_p$

$m_i \rightarrow$ weight fraction of the constituent

60% A & 40% B

$C_0 = 0.6 \times C_{0A} + 0.4 \cdot C_{0B}$

There are different methods to do that but we will go with the simplest one very simple method interpolation method one of the interpolation method, so what we can do is we can just take c0 these shock parameters c0. We can take summation of m i c0 i and similarly s = summation of m i s i what is this mi, mi is the weight fraction of the constituent.

So you can use it from mixtures and you can use this for alloys although alloys is not a it is just a approximation which is not very may not be very accurate. So basically c0 and s you can understand this is the thick for the linear relationship equation of state c0 s U p. So these we can do it like that and also the density will be Rho0 summation of m i Rho0 i, so that means if you have a alloy with let us say 60% A and 40% V if we know the c0 and s for this A and B.

So then what we can do is like c0 for the alloy will be 0.6 multiplied by c C0 A + 0.4 multiplied C0 B. So this is similarly you can do it for s or even for density, so this is very simple but there are other rigorous methods involved for this mixtures and alloys.

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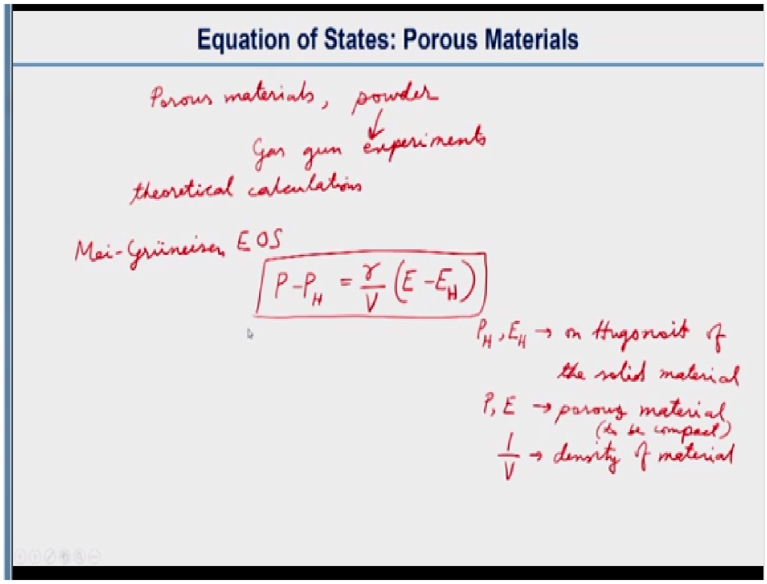

Equation of States: Porous Materials

Porous materials, powder

↓

Gas gun experiments

theoretical calculations

Mei-Grüneisen EOS

$$\boxed{P - P_H = \frac{\gamma}{V}\left(E - E_H\right)}$$

P_H, E_H → on Hugonoit of the solid material

P, E → porous material (to be compact)

$\frac{1}{V}$ → density of material

We just want to talk about this EOS for porous materials let us say for powders porous material powder can be considered as a porous material. So people use gas gun experiments for powders but we can also use theoretical calculations. So here we can use the Mie-Gruneisen EOS which will be P - P H = gamma B V E – EH, so this H is for let us say that is for the solid material.

So PH and EH on Hugonoit of the solid material the Hugonoit curve of the solid material the same solid material of the which the powder is of, so solid material and then PE for porous material or powder let us say porous material. And 1 by V is the density of the solid material density of material, so basically these are the relations of, so this is the porous material let say we want to compact it to be compacted.

So you want to compact the material using pressure and then using shock pressure, so this is the relation we need to follow.

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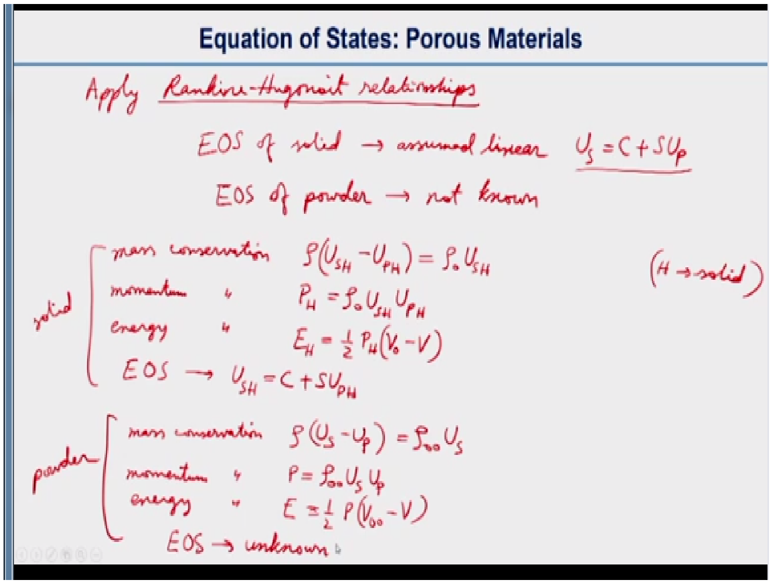

Equation of States: Porous Materials

Apply Rankine-Hugoniot relationships

EOS of solid → assumed linear $U_s = C + SU_p$

EOS of powder → not known

solid
- mass conservation $\rho(U_{SH} - U_{PH}) = \rho_0 U_{SH}$
- momentum " $P_H = \rho_0 U_{SH} U_{PH}$
- energy " $E_H = \frac{1}{2} P_H (V_0 - V)$
- EOS → $U_{SH} = C + SU_{PH}$

(H → solid)

powder
- mass conservation $\rho(U_s - U_p) = \rho_{00} U_s$
- momentum " $P = \rho_{00} U_s U_p$
- energy " $E = \frac{1}{2} P (V_{00} - V)$
- EOS → unknown

And what we can do is we can use we can apply Rankine Hugonoit relationship that those are nothing but the conservation equations EOS of solid. Let us say we assumed linear that means E EOS = c + s U p and then EOS of the powder that the porous material of that is not known. So we want to know this EOS of powder, so we will use you will apply the Rankine Hugonoit relationships and also we have the EOS of the solid.

So how you can do let us say for the solid we will write first solid, so mass conservation which will be you must remember this equation you already found some equations. So we are not going to show you how we got that but I hope that you already you know we had an earlier discussion we mentioned this. So this is shock wave velocity, so H is for solid the subscript H is for solid and then momentum conservation.

And then energy conservation some momentum conservation is pH is = Rho0 U s H u p H then energy conservation is specific internal energy well to half of pH V0 - V and then EOS of the solid is U s H c+ s U p H. Similarly for the powder what we get is a mass conservation is a rho U s U p - = rho 00, so double knot we use for the powder.

So similarly for momentum and then energy conservation momentum is p = rho 00EOS U p, E = half of p V 00 - V and then EOS, EOS is what, so EOS is unknown equation of state is unknown.

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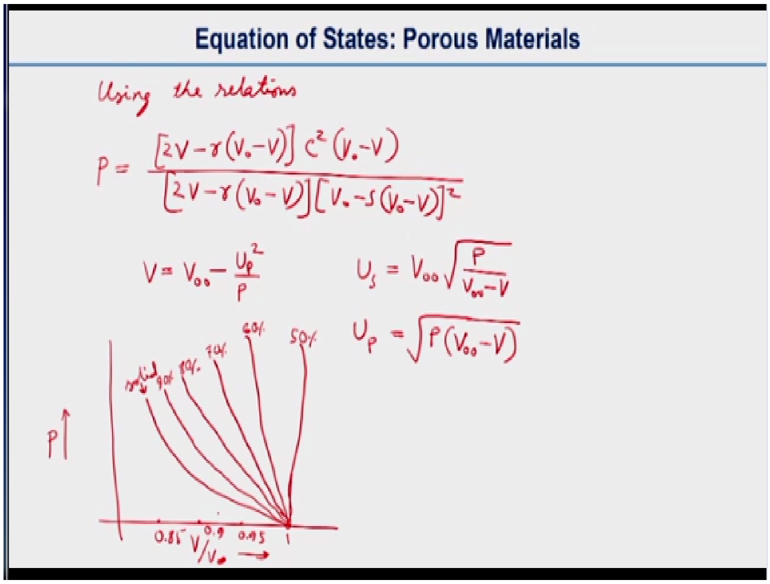

Equation of States: Porous Materials

Using the relations

$$P = \frac{[2V - \gamma(V_0 - V)]\, c^2 (V_0 - V)}{[2V - \gamma(V_0 - V)][V_0 - s(V_0 - V)]^2}$$

$$V = V_{00} - \frac{U_p^2}{P} \qquad U_s = V_{00}\sqrt{\frac{P}{V_{00} - V}}$$

$$U_p = \sqrt{P(V_{00} - V)}$$

So using this relations we are not going to derive it using the relations described in the last slide. so we can find a relationship between p and V pressure and V which is a very big expression twice V - gamma that Mie-Gruneisen constant this c square V0 - V + twice V gamma V0 V V0 – s, V0 - V square and where this V you can V has can be related with the particle velocity like that and here U s is p V 00 V and then U p = p V 00 V.

So if we have this relationship in a plot that is a specific volume V by V0 and x axis V by V0 and the pressure on this x is let us say we have a powder which specific volume 1.95, 0.9, 0.85, so what will happen is if we can draw the solid curve like this, this is solid. So if we take some other curves of the powder, so the powder curves will look like this I will tell you what are these curves let me first draw it.

So this is for let us say for 90% relative density of the powder let us say 90%, 80% and 70%, 60 and 50% that means this is 50% porous. So this is for solid and others are powder, so it will look something like this, so that the b plots are not really clear here but you can check it from your the textbook. So this is basically what we talked about the equation of state for porous material.

So we will discuss in the next class we will discuss about a little bit about a temperature rise due to shockwave and also we will talk about the shock wave interaction reflection in the next lecture, thank you.