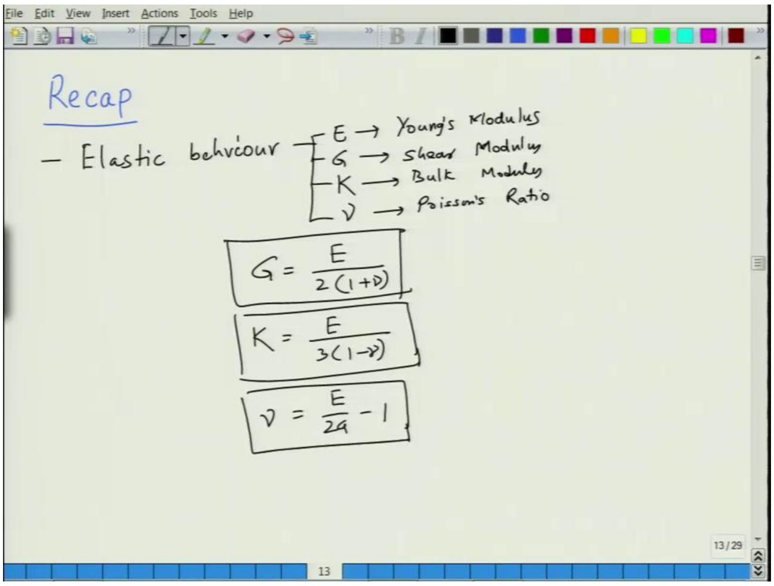
Properties of Materials (Nature and Properties of Materials: III)
Professor Ashish Garg
Department of Material Science and Engineering,
Indian Institute of Technology Kanpur
Lecture 10
Atomic Basis of Elasticity

So welcome again to the new lecture of this course, Properties of Materials. So let us just do a brief recap of what we did in the last lecture.

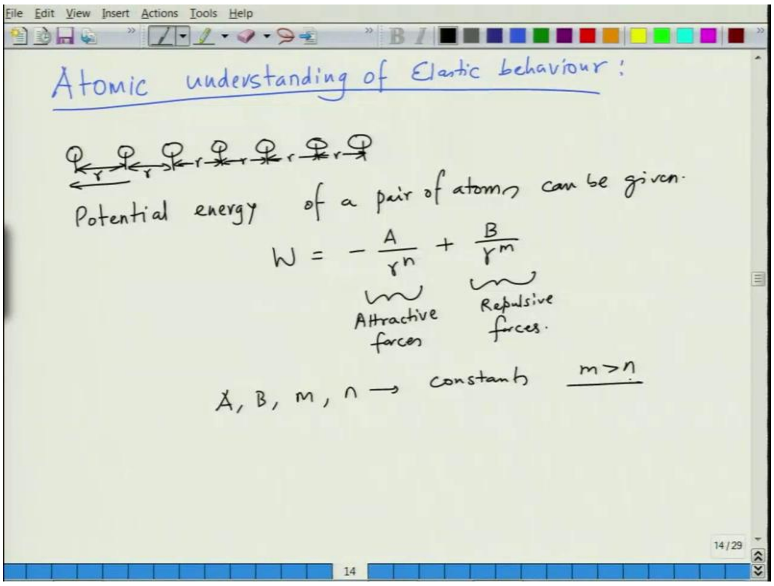
(Refer Slide Time: 0:22)



So in the last lecture we learnt about essentially, and we finished the discussion on elastic behavior, mainly to do with the discussion of properties E, G, K and nu. So this is Young's modulus, this is shear modulus, this is bulk modulus and this is poisson's ratio. And the relation between the three was, so G is related to E, as G is equal to E divided by 2 into 1 plus nu.

We can right K, this is equal to E divided by 3 into 1 minus nu. And if you eliminate K from this, we can write nu in the form of E and G, this is E divided by 2G minus 1. So these were the three relations that we worked out in the last lecture. So this was a basic, a very brief primer about what elastic properties are.

(Refer Slide Time: 01:44)

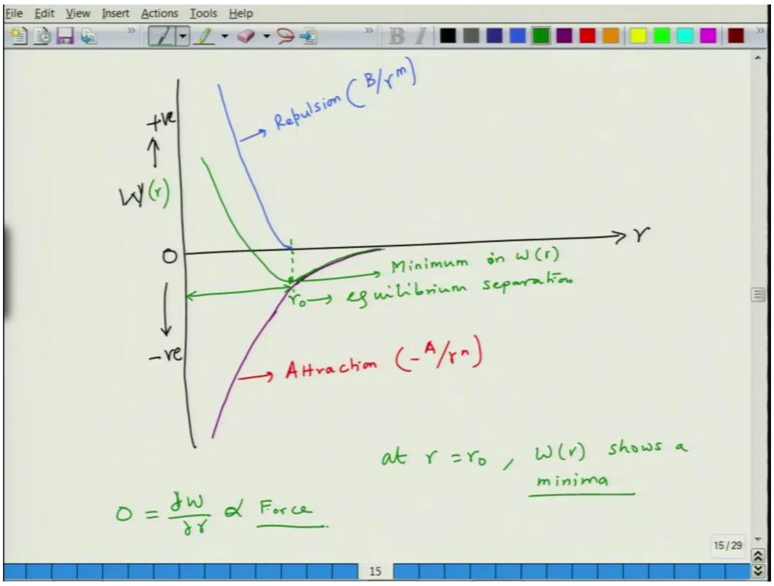


Now in this class we will look at atomic understanding of elasticity, of elastic behavior. So when you have these two, when you have a material, this row of atoms, so the question is what determines the equilibrium distance between the two atoms and we see that in most materials, in crystalline materials, the atoms have equilibrium separation, which is called as lattice parameter.

So we will see that most materials have atoms located at a very well defined distance r or r naught, let us say, and why is that so. And this is because of potential energy minimization. So potential energy of a, let us say, a pair of atoms can be expressed as, so potential energy between the two atoms can be given as, let us say, W is equal to minus of A divided by r to the power n plus, plus of B divided by r to the power m.

So here the first term is negative term, which depicts the attractive forces between the two atoms and this depicts the repulsive forces. And this is what basically balances the atoms. So there is a certain distance as we will see at which this energy is minimized. So here A, B, m, n, these are all constants and m is greater than n.

(Refer Slide Time: 03:54)



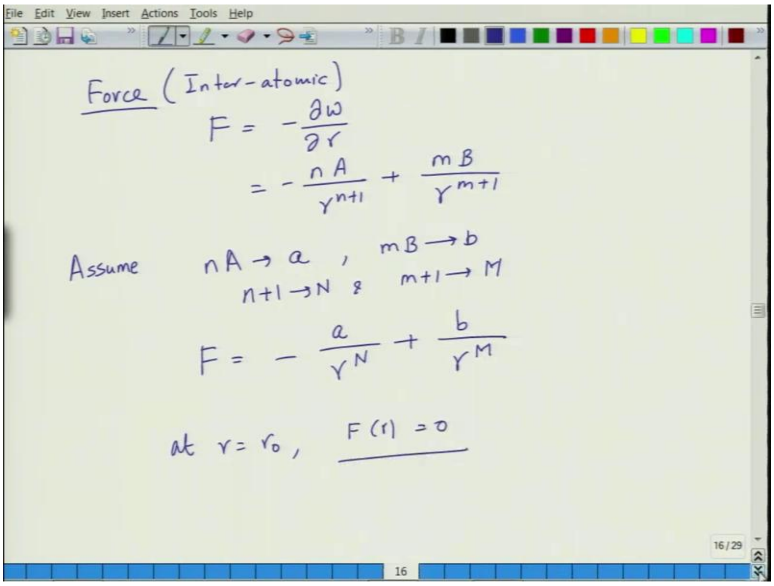
So, now when you plot this potential energy, so let us say, when we plot this potential energy as a function of distance, this is 0, so this would be positive, and this would be negative. So naturally the positive part will be defined as repulsion. So this will depict repulsion and it is characterized by the term B divided by r to the power m.

And then we have the next term which is the attraction, which is, which goes something like this. And so this is, this is A divided by r to the power n, minus of A divided by. And if you make a composite plot, a composite plot shows, a composite plot is something like this, it follows this. And at certain separation which happens to be the same point at which repulsive forces die much more quickly, because m is much larger than n.

So round about at the point where repulsive force is also weaken is the point which is the distance r naught, which is the equilibrium separation. And this is where potential energy is minimized. So this where the minima, you can say the minimum in w r. So this is basically w as a function of r, which gets minimized at this particular point.

So at r is equal to r naught, w r shows a minima. What does it mean? The derivative of w r which is del w by del r, this is equal to basically force, it is proportional to force. So which means where you have a minima, if you take the derivative, derivative will be equal to 0 and which means the force at that point is equal to 0. What it means is that at, that is the point at which repulsive and attractive forces counterbalance each other and they balance each other.

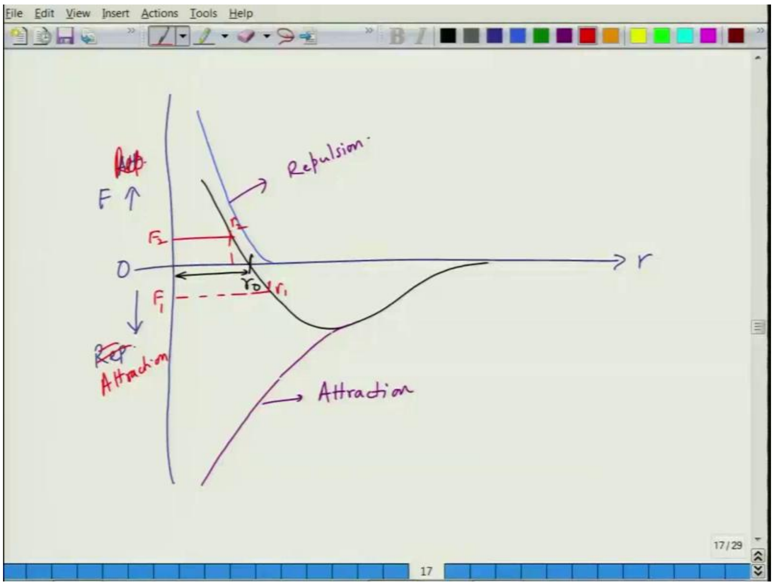
(Refer Slide Time: 06:40)



So one can derive the force, so now if we write the force, the force can be written as, inter-atomic force, let us say, is equal to minus of del w divided by del r. This equal to minus of nA divided by r to the power n plus 1 and this becomes mB divided by r to the power m plus 1.

So let us assume that small nA is another constant a, and small B is another constant b and n plus 1 is equal to N and m plus 1 is equal to M. If we do that, then what we write this F as minus of a divided by r to the power N plus b divided by r to the power M. And basically at r is equal to r naught, F r is equal to 0.

(Refer Slide Time: 07:56)

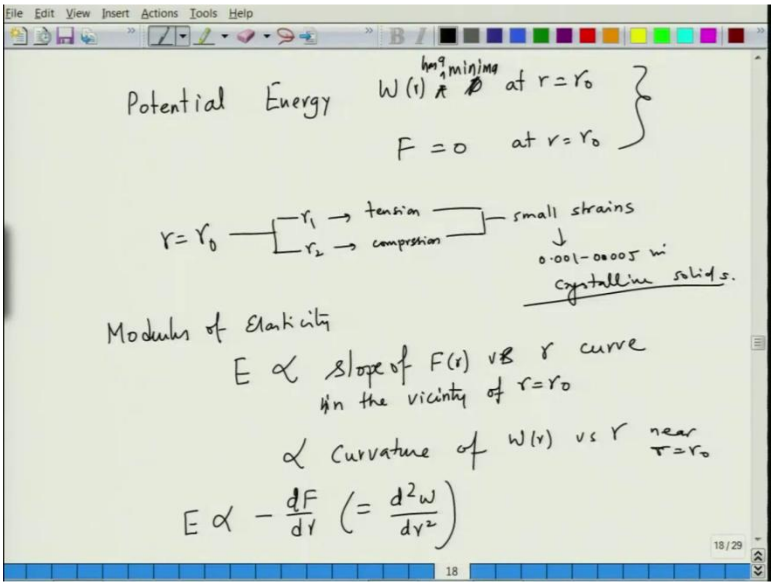


So essentially when you plot the force now, so this is attractive, this is repulsive, this is r. So now when you plot the, and this is the place where the force is equal to 0 and this is r naught and if you plot the other two component of the forces, the repulsive forces will go something like this and the attractive forces will continue to have this kind of, so this is repulsion and the force is 0 at r is equal to r naught.

Now if you wanted to move away from this particular point, let us say you wanted to go here, which means you will have to apply an extra repulsive force. This is F, let us say, I do not know r 1, you will have to apply a force F1 to go to higher distance, which means you will have, this is repulsion, I am sorry, this is attraction, my apologies. So you will have to apply attractive force or you can say compressive force to go to r1.

If you wanted to go to this particular point, let us say, r2 then you will have to apply a force F2, which is the repulsive force or the tensile force. So you will have to apply an extra energy in order to move away from the equilibrium point at r naught. So this is what basically the gist of this is now.

(Refer Slide Time: 09:54)



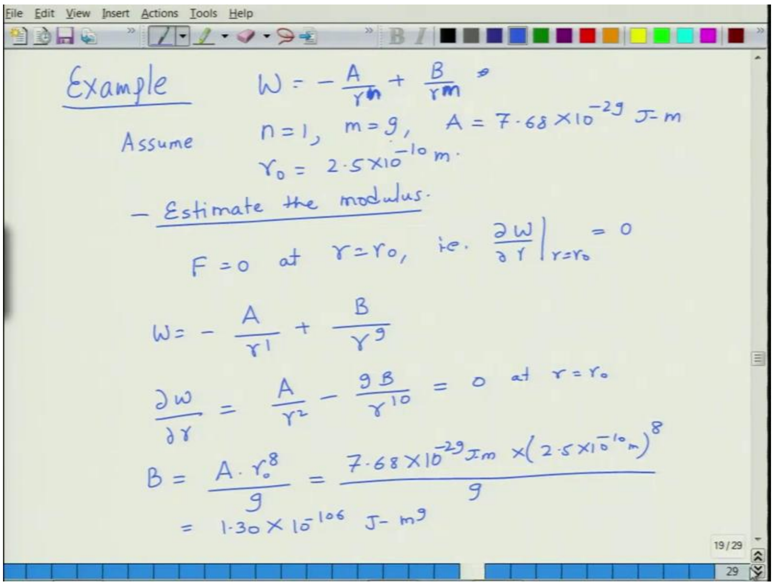
Potential energy, sorry, shows a minimum, has a minima at r is equal to r naught and F is equal to 0 at r is equal to r naught. This is what the summary of previous point is.

Now this, in crystalline solids, generally when you want to go to, so when you want to go from r is equal to r naught to let us say and you apply tension or compression, r1 or r2, let us say, this is tension, this is compression. Since the force applied can be quite substantial, the strains are generally very small. So it leads to generally extremely small strains, elastic strains, because when you take it to this point it goes back, when you take it to this point it comes back, it is like a spring action.

So when you apply these tensile and compressive forces, the atoms tend to get back to their position as soon as you release the load. So these strains are very small strains generally of the order of 0.001 to 0.005 in crystalline materials, especially metals and ceramics and polymers, they can be quite large.

And the modulus of elasticity E is basically proportional to the, or you can say is proportional to the curvature of w r versus r near r is equal to r naught. So essentially you can say that E is proportional to minus of dF by dr, which is we can say is also equal to d2w divided by dr2.

(Refer Slide Time: 12:42)



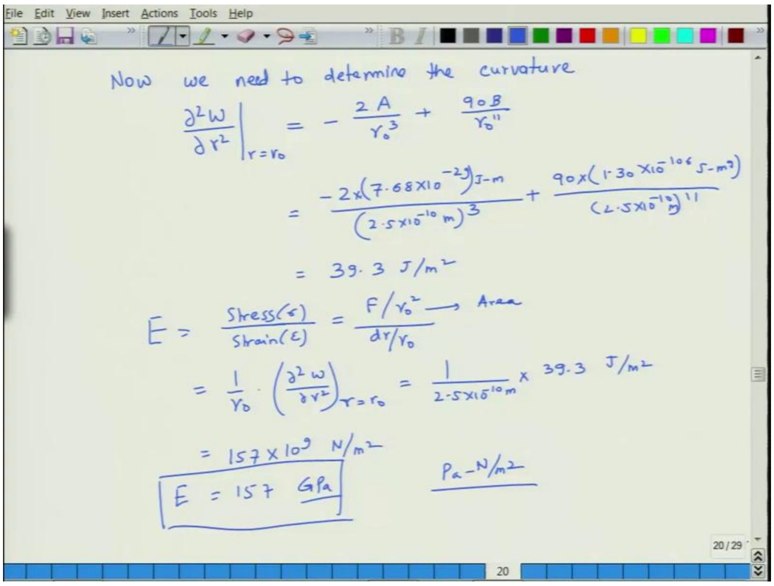
So let us take an example in which we would like to calculate the modulus for a given material. So let us take an example that will make things little bit more clear. So we know the formulas. Formula is for potential energy is W is equal to minus A divided by rm plus B divided by rn, sorry, rn and rm. So this will be, so let us say, assume, n is equal to 1, m is equal to 9 and value of A being 7.68 into 10 to power minus 29 joule meter and let us say the value of r naught is given as 2.5 into 10 to power minus 10 meter. This is the data that is given to you. You need to calculate the modulus.

So estimate the, so how do we now determine the modulus? First thing that we know we are given r naught. When is r is equal to r naught, r is equal to r naught when the force is equal to 0 that is the derivative of w with respect to r will be equal to 0. That will help us determine the value of, so we can see we have a value of n, we have a value of m, we have value of A, but we don’t know value of B. That will help us to determine the value of B.

So first thing first is force is equal to 0 at r is equal to r naught, that is del w by del r at r is equal to r naught is equal to 0. So when we do this, so we derive this. So this makes it A divided by, so now w can be written as minus of A divided by r to the power 1 plus B divided by r to the power 9. So del w by del r will be equal to A divided by r square minus 9B divided by r to the power 10 and this is equal to 0 at r is equal to r naught.

So now B will be equal to, in that case, A into r to the power 8 divided by 9. So we put in the value of A that is 7.68 into 10 to power minus 29 joule meter into r to the power 8 and this is r naught essentially, so we can say it is 2.5 into 10 to power minus 10 meter to the power 8 divided by 9. So this will turn out to be 1.30 into 10 to the power minus 106 joule meter to the power 9. So we can see that this is 1 meter, this is meter to the power 8, this will become meter to the power 9. This is the value of B.

(Refer Slide Time: 16:13)



So now we need to determine the curvature. So curvature is given as second derivative del 2 w by del r square that is equal to r is equal to r naught and if we do that differentiation again, we get minus 2A divided by r naught to the power cube plus 90B into r naught to the power 11.

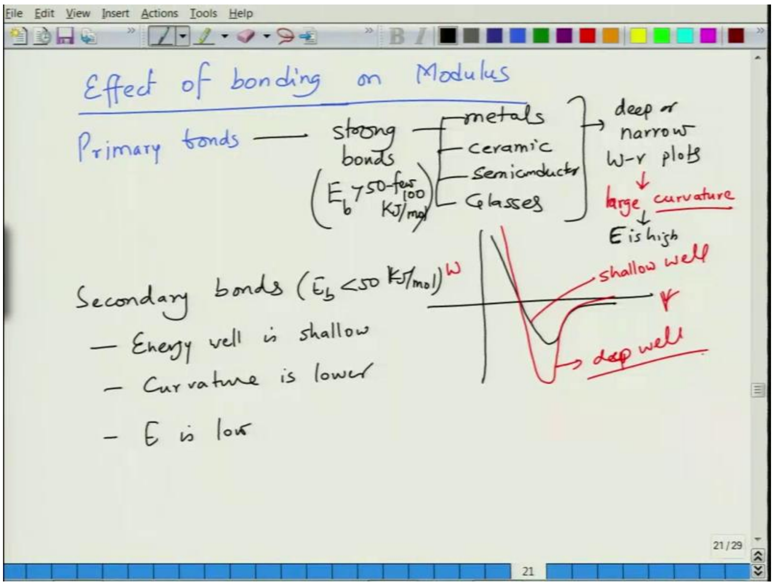
So if you now plug in the values, what you get is minus 2 into 7.68 into 10 to the power minus 29 that is joule meter divided by 2.5 into 10 to the power minus 10 meter to the power cube, to the power 3 plus 90 into 1.30 into 10 to the power minus 106 joule meter to the power 9, this is 90B divided by r naught, which is 2.5 10 to the power minus 10 to the power 11 and this is in meter. So we can see that you will get something into, in the form of joule per meter square, because of, so this will give rise to a value 39.3 joules per meter square.

So modulus is now given as stress divided by strain, sigma divided by epsilon. What is stress, stress is force per unit area. So, let us say, the force is F and area we approximate as r naught square. So this is area, just a approximation. And strain is, let us say, dr divided by r naught. So dr, r naught is the original length and dr is the small extension that you provide of infinite estimate d small. So this becomes equal to 1 over r naught into del 2 w by del r2 at r is equal to r naught.

If that is the case, so this is just approximation, in the vicinity of r naught that is why we have taken r is equal to r naught. So this is 2.5 into 10 to minus 10 meter into 39.3 joule per meter square. So this will become 157 into 10 to the power 9 Newton per meter square or 157 GPa, 1 pascal is equal to Newton per meter square. Pascal has more conventional value to represent modulus versus stress.

So modulus is calculated at, as 157 giga pascal as we have seen from this data. So I hope it is clear that how do you estimate the modulus from the potential energy calculations by using simple analysis. Of course, this is grossly simplified, but nevertheless it gives you the gist of what the relation between modulus and potential energy is.

(Refer Slide Time: 19:59)



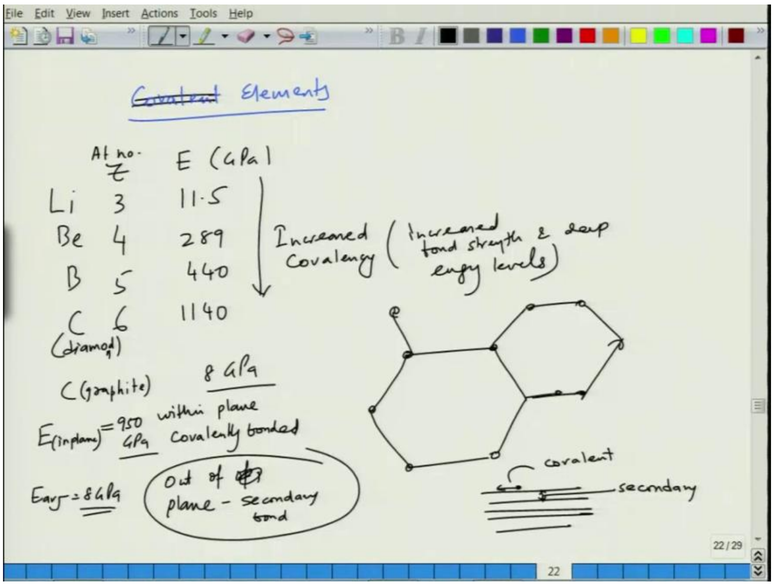
Now let us look at, in the last lecture then, we, in the end, we talked about relation of bonding with modulus. So based on the bonding, we know there are different kinds of materials. So we have primary bonds, which are strong, basically in metals, most metals, except soft metals, ceramics, also semiconductors, glasses, these will have strong bonds. So strong bonds will generally mean strong bonds, which means energy of the bond will be generally more than 50 and it could be few 100 kilo joule per mole.

So when you have this kind of bond energy and this gives rise to deep or narrow w r plots. So essentially the potential energy plot would be, so if you wanted to plot something, something like this, so it has not come out very well, but what I mean is that something like this, so this is a shallow well, this is deep well.

So you can see that, when this leads to basically change in the slope as well as curvature, so this is w r. So deep well will mean you will have large curvature, higher slope, higher slope will lead to larger curvature.

On the other hand, you have secondary bonds, like hydrogen bonds, van der waal bond and so on and so forth for whom the bond energy is generally less than 50 kilo joule per mole, smaller than 50 in most cases, maybe above 10, 20 or even 1 or 2. In those cases, the energy well is shallow, curvature is lower and hence E is low. So here E is high and here E is low. And this is very much related to the data.

(Refer Slide Time: 23:03)

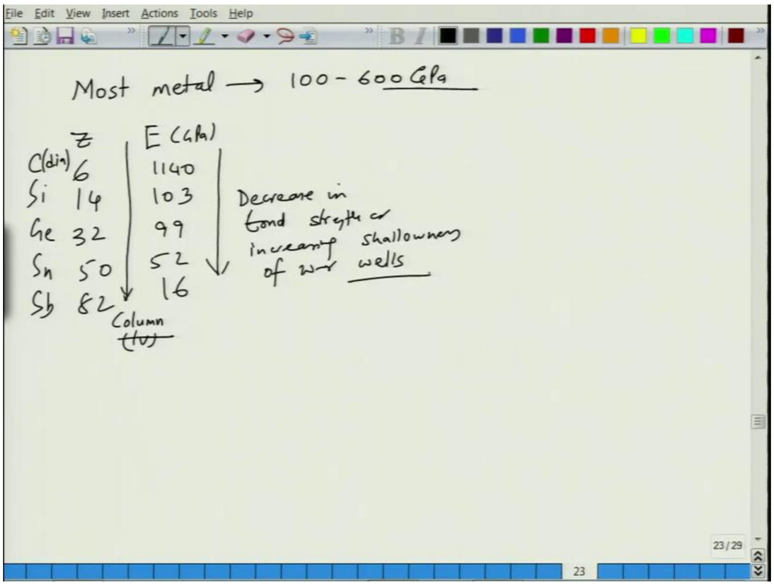


So if you look at, for example, materials like, if you just consider the covalently bonded elements. So if you consider the case of. So you have z, which is the atomic number, 3, 4, 5, 6, what does it belong to? This is lithium, this is beryllium, this is boron and this is carbon, or let us say just elements, just the plane elements. Now the modulus value, the E value in GPa goes from 11.5 to 289 to 440 to 1140 and this is related to increased covalency, basically increased bond strength and deep energy levels.

If you compare, for example, this is diamond form of carbon. Now the same thing if you do for graphite, which has secondary bonds, this shows a modulus of 8 GPa awfully small, but graphite has a structure, which is hexagonal structure. So within these layers, it is and so on and so forth. So it is within the plane covalently bonded and out of plane secondary bond. So these are graphite plate, plaques. So this is, let us say, secondary bond and within the plane you have covalent bond.

So within the plane, so if you take E in plane, in plane E value of graphite is 950 GPa, very much close to diamond. So within the plane it is very strong. But if you look at the average value considering all the directions powder of graphite, basically polycrystalline form of graphite, then it falls to 8 GPa and this is the contribution which comes from these out of plane secondary bonds which are very, very weak bonds.

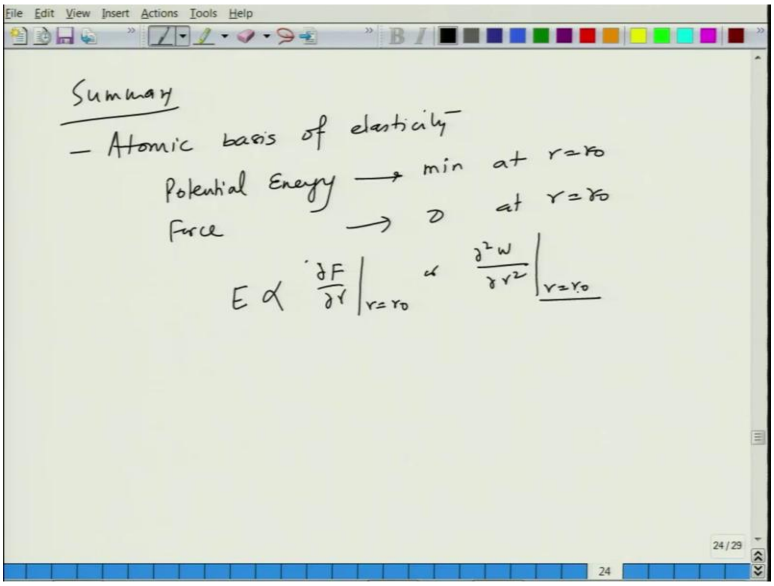
(Refer Slide Time: 25:46)



If you look at most metals, most metals have modulus which is between 100 to 600 GPa. So now let us also compare what happens when we go down the row. So if you plot, for example, z is equal to 6, 14, 32, 50, 82. So you go from carbon to silicon to germanium to tin to antimony and this is diamond basically, and elastic modulus varies from, so this is going down the row, going down the column, sorry. So this is column IV.

So you can see that it changes from 1140 to 103 to 99 to 52 to 16 and this is again decrease in bond strength or increase in shallowness of w r wells. So which means the curvature reduces as a result the modulus goes down. You can also compare various other materials which are metals and ceramics and we will do that comparison in the next class. We are running out of time now. So we will stop here.

(Refer Slide Time: 27:14)



What we have done in this lecture is basically, so just summary, so in this lecture what we have done is we have established an atomic basis of elasticity. So basically what we have looked at is the potential energy and force. At equilibrium separation potential energy is minimum and force is 0 at r is equal to r naught. And the modulus is related to the slope of force versus distance plot or curvature of potential energy versus distance plot.

So higher the curvature, higher the slope is, more the modulus is, which means deeper the wells are, the steeper the wells are, more the curvature is, more the bond energy is, more the modulus is. This is what we have seen and we saw a few examples for, for example, group IV elements or just lithium, beryllium, carbon and some other elements.

So what we will do in next class is, we will further develop on this aspects of elasticity before we close this. Thank you.