Introduction to Materials Science and Engineering
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Lecture – 60
Free surface or external surface of the crystal

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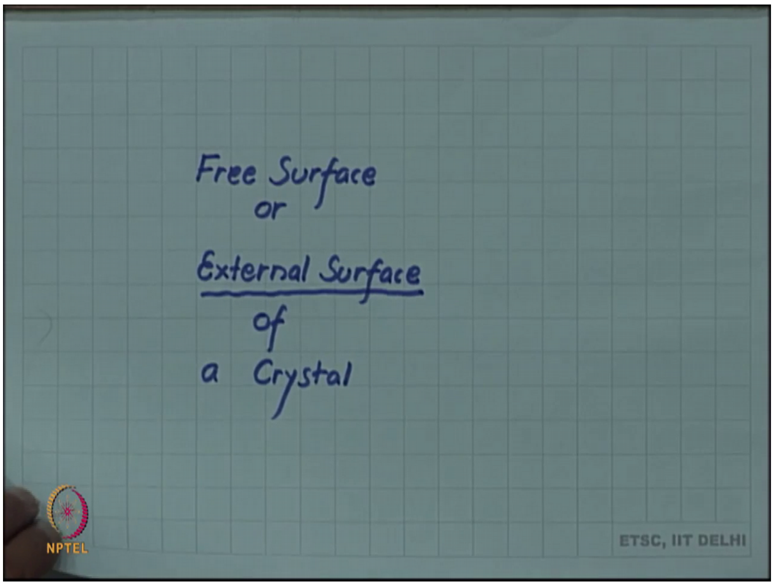

So we have started our discussion on surfaces and interfaces in crystalline solids. Now, we will take a particular kind of surface which is always present in all crystal and that is it is external surface. So, since all crystals will be finite, there will always be an external surface of that crystal and this external surface is itself a kind of defect.

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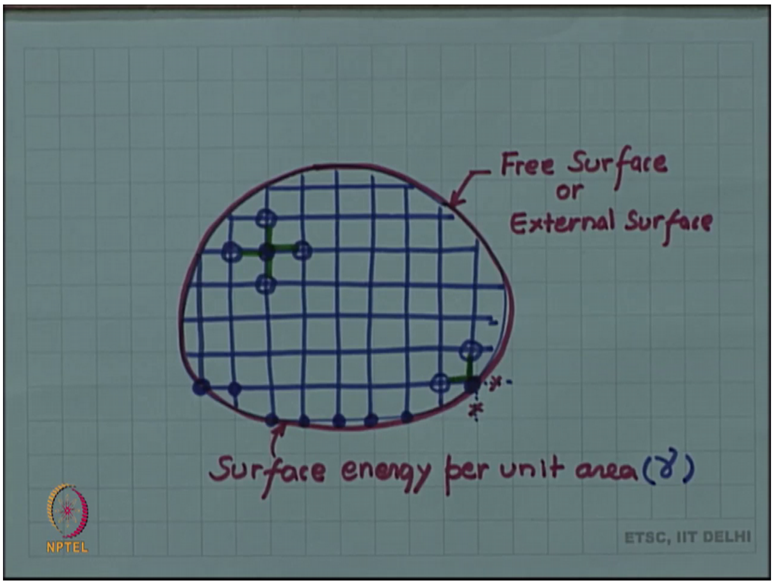

Because, you can see if we have, if we have any crystal bounded by a surface, inside we can have nice perfect lattice, even if it is free. We have already discussed, it cannot be free of vacancies if it is at a finite temperature greater than absolute 0 because vacancies are in thermodynamic equilibrium in crystal.

But for the moment, if we say it is free of vacancies and it is free of dislocations; is still, since it cannot be infinite there will obviously be a boundary; there will be an external boundary of the crystal, the external boundary and that external boundary itself since it breaks the lattice periodicity at that position. So, this free surface is a defect. So, this is a free surface or external surface. An every external surface actually leads to breaking of bonds, you can see it leads to breaking of bonds.

So, a given atom in this 2 dimensional model, in this 2 dimensional model, a given atom has 4 nearest neighbors; this central atom has 4 nearest neighbors. So, it forms bond with 4 of these. So, every atom is forming, a every inside atom is forming bonds with 4 nearest neighbors; however, if you look at a surface atom, if you look at an atom sitting on the surface, let us say here then it has only 2 nearest neighbors; 2 nearest neighbor. It has only 2 bonds. Other 2 bonds which it was supposed to form, if the crystal was infinite are now actually broken because it is sitting on the surface.

So, these 2 other neighbors are lost and you can think of that breaking of bonds requires energy. So, because of the breaking of these bonds, extra energy is provided to the crystal and that energy resides in this surface atom; integrated over this entire surface, the higher energy of this surface atom is what is called the Surface energy of the crystal or the surface energy of the surface. So, this will have a surface energy per unit area of the crystal.

So, actually all the atoms which are sitting on the surface have lost certain number of bonds and that is what is giving us the extra energy to the surface. So, surface energy per unit area. We will use the symbol gamma for this quantity.

Now, in terms of this bond breaking model, we can actually develop formulation for this surface energy. So, that is what we will do now.

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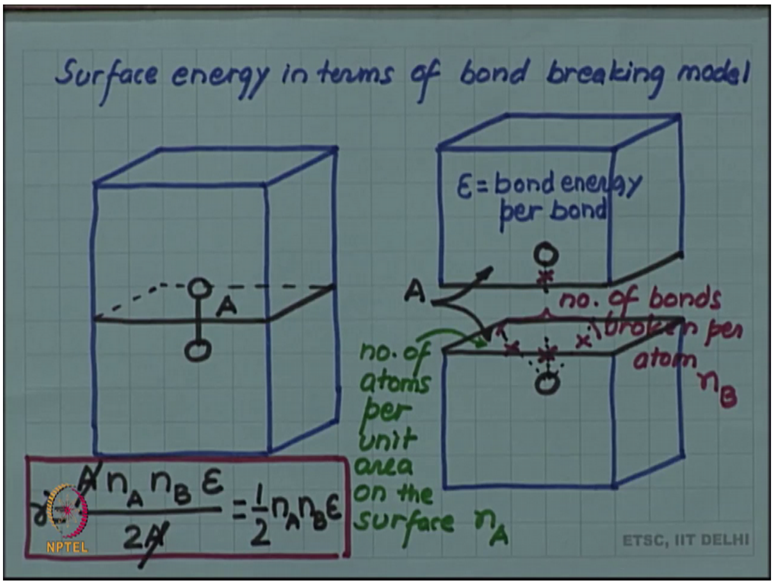

The surface energy in terms of bond breaking model or bond breaking model of surface energy, you can say this. So, let us think of this as, let us begin with a crystal. So, I am starting with a block of crystal. This is my block of crystal; it already has a lot of free surfaces, but let me try to create a new free surface by breaking this crystal into 2.

So, I cut this crystal at this plane into 2 halves. So, what I get is one crystal, a broken this on this black plane. Now, for atoms sitting on this plane, since we created initially let us think of think of an atom here and an atom here, which let us say were bonded through this bond. But now that atom sitting here, these 2 are bonded, but these bonds are now broken; these bonds are now broken because we have created a new surface.

So, these bonds are broken. So, that much of extra energy is provided to break this bond. And we will like to calculate the energy of this surface in terms of these broken bonds. So, the parameters which we require for this is, one thing is how many atoms are there on this surface. So, we require number of atoms per unit area on the surface, on the free surface; how many atoms are there on that a surface.

Now, I have shown that an atom is losing only 1 bond, but it is quite possible that an atom is bonded to more than 1 atom on the other side, more than 1 atom on the other side. So, you will have more than 1 bonds breaking. So, another quantity which you need is number of bonds broken, number of bonds broken per atom, number of bonds broken per atom on the surface. So, this will be another quantity.

So, let us call this quantity number of atoms per unit area as n A and let us call this quantity number of bonds broken per atom as n B. And of course, the energy which we are going to provide in breaking this bond is the bond energy. So, the third important quantity which let us call that epsilon is the bond energy is the bond energy per bond. So, since across an area A, across an initial area A, let us see if this was the initial area A, across the initial area A, I will break all the bonds of these n A atoms and then I will create this free surface. But if I break the bonds over an area A, I have created 2 free surfaces an area A above and an area A below.

So, I have created 2A surface area. So, let us now look at the energy required. So, there were any atoms per unit area, I multiply that by area A over which I am breaking it. So, A times n A is the number of atoms sitting on this area each of them is having n B bonds. So, this is the total number of bonds involved which I have to break to create these 2 surfaces.

And then each bond required epsilon energy to break it. So, I have supplied this much energy to break all the bonds over this area. But since I have to find out this a surface energy per unit area, I divide it by the area creating, but the area created is 2A. So you can see, I get a simple formula for the surface energy per unit area gamma as half n A n B epsilon, half n A n B epsilon. So, this will this is our final formula for the surface energy. We will apply it for some a special cases to find the surface energy of different crystals.