

STUDENT:

Hello, everyone. Today, I'm going to talk about a very important model, analyze the energy band of a crystal, that is the tight binding model. Before I talk about tight binding model, let's now take a look at free electron model. The potential energy of free electron can be considered as zero, so the Hamiltonian of the free electron system is without the potential term. And the waveform function can be simply written as a plane wave.

By substituting the wave function into Schrodinger equation, we can gather energy dispersion relation, which is a parabola in one dimension case. And we usually form the parabola into the first Brillouin zone. And this is the reduced Brillouin zone. And in this figure, we can see that the first band is at the bottom of the parabola. And the second band and third band, fourth, and so on.

Similar to one dimension case, the energy of three dimension case is proportional to $k_x^2 + k_y^2 + k_z^2$. For a given energy, the equal energy surface forms of a sphere. And if the energy is equal to the Fermi energy, the states inside the sphere will be occupied by electrons. Now let's look at the two hydrogen atom system.

When the two atoms are very far from each other, the wave functions don't overlap. As the two atoms going towards each other, the electron of atom a starts to build existence of atom b and the wave functions start to overlap. We can see that when the two atoms are close, two new orbital are created. One is the bonding orbital and the other one is the antibonding orbital. For the bonding orbital, we can see the probability to find the electron between the two atoms is larger than before. And in the antibonding orbital, we can see that in the middle of the two atoms, the probability to find the electron is zero.

The overlap of the wave function in bonding orbital, leading to a higher banding energy, which leading to a more stable state. So the bonding orbital is the ground state of the system. And antibonding orbital is excited state of the system. Let us now talk about the tight binding model. Assuming the potential of a single atom is U , then the Schrodinger equation can be written like this.

We now consider the effect of other atoms as perturbation, as we have seen in the last slide. Each energy level of each atom split into two in a two hydrogen atom system, the degeneracy of each energy level is two. For a system of n atoms, the degeneracy of each energy level is

n. From the perturbation theory, the wave function for degenerative system can be written as a linear combination of degenerate states.

And if a_j in the expression is equal to the expression on the right, the function satisfies the block theorem. We can also write the first order correction of the energy, which is the diagonal interest of the Hamiltonian matrix. Now we only consider the integration of the atom itself and its nearest neighbors. So we can further simplify the expression and the ways we set $j=0$ as the integration of the atom itself. And j as the integration of its nearest neighbors.

Note that the integration is determined by the overlap of the two wave functions. The more they overlap, the wider the energy band is. And finally, we get our final dispersion relation of tight binding model. Now let's see what has happened after applying the tight binding model to a one dimensional system, assuming that the distance between atoms is a , each has only in a one dimensional atom chain has two nearest neighbors.

So the sum of the expression has two components, where ρ_n equals to a and the minus a . By using the Euler's formula, the dispersion relation can be written as a trigonometric form. The figures show the first two bands of a one dimension system for free electron model and tight binding model. We can say that because of the inference of nearest neighbors, distortions appear at the boundaries of the Brillouin zone, and leading to the opening of a bandgap, which is quite different from the free electron model.

In three dimension cases, the dispersion relations are more complicated. Let's now take a look at the dispersion relations of these three kinds of 3D lattices. For a simple cubic lattice, there are six nearest neighbors of one atom. So the sum has six components. And we can get the dispersion relation like this after simplifying. While for body-centered cubic, there are eight nearest neighbors, which leads to an expression like this. For face-centered cubic, they are 12 nearest neighbors. And we get a dispersion relation like this.

So what do the relations on the last slide look like in the first Brillouin zone? In 3D crystals, we can calculate the reciprocal primitive vectors by using the formula below. The reciprocal lattice of simple cubic is also a simple cubic. And the reciprocal lattice of a body-centered cubic is face-centered cubic, while the reciprocal lattice of a face-centered cubic is body-centered cubic.

The first Brillouin zone is defined as the region inside the perpendicular bisectors of the segments linking a point to its nearest neighbors. As we know, the reciprocal primitive vectors

we can plot the first two Brillouin zones of these lattices. These graphs show the Bravais lattice in real space and its energy dispersion in the reciprocal space.

For a simple cubic, the first Brillouin zone is a cube. And when the energy is small, the equal energy surface looks like a sphere, like a free electron case. As we can see, when the energy goes up, distortion begins to appear. And when the energy reaches the boundary of the first Brillouin zone, openings or holes appear at these boundaries.

In these figures, we can see that in the first Brillouin zone of BCC lattice, similar to a simple cubic lattice. Distortion gradually appears as the energy goes up. And the surface is no longer close to the surface at the boundaries as the energy goes higher and higher. And sodium is a BCC crystal, because there is only one valence electron per sodium atom. So the Fermi surface is pretty far away from the boundaries and the shape of it is nearly a sphere, which is like this.

In FCC crystals, such as copper and gold, their Fermi surface can be well-described by the tight binding model. At the hexagonal faces, holes appear. Well, because the distance is further between the Fermi surface and the square faces. So these areas of the surface won't extend and contact with the squares. Well, I hope that through this short video you can understand what the tight binding model is and how we use it as a tool to explain the phenomena in a real material. Thank you for your watching.