Metal-semiconductor interfaces

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Outline

1. Surface state
2. Semiconductor surfaces
3. Work function measurement
4. Metal-semiconductor interfaces
Surface state

- The wave function for the electron, labeled by \((n,k)\) where \(n\) is the band index and \(k\) the electron wave vector
  \[ \varphi_{n,k}(r) = u_{n,k}(r) \exp(ikr) \]
- Two types
  1. Surface resonance - the wave function is bulklike inside the solid and decays exponentially from the surface to vacuum
  2. True surface state - the wavefunction decays to zero on both sides of surface.
According to Schrödinger equation

$$\left[-\frac{d^2}{dz^2} + V(z)\right] \varphi(z) = E \varphi(z)$$

$$V(z) = -V_0 + 2V_g \cos gz$$

Solve it, we get

$$\varphi = e^{ikz} \cos \left(\frac{gz}{2} + \delta\right)$$

$$E = -V_0 + \frac{g^2}{4} + K^2 \pm \sqrt{g^2K^2 + V_g^2}$$
• There is the usual energy gap at \( K=1 \), the zone boundary.
• \( E \) can be a continuous function of \( K^2 \) if we allow negative values of \( K^2 \). In the bulk, these solutions are not allowed because they lead to infinite wave amplitudes as \( z \) approaches infinity.
Now we consider the case in which we terminate a solid with a surface as below.
Now we consider an n-type semiconductor at thermal equilibrium at temperature $T$ above absolute zero.
The variation as a function of distance in the space charge region can be obtained by solving the poisson equation.

\[
d\frac{d^2V}{dx^2} = -\frac{\rho}{\varepsilon\varepsilon_0}
\]

Now, we use depletion approximation

\[
\rho(0 < x < x_D) = eN_D \\
\rho(x > x_D) = 0
\]

Then we get

\[
V(x) = -\frac{eN_D(x - xD)^2}{2\varepsilon\varepsilon_0}
\]
1. The Fermi level is flat.
2. The upward bending of all the bands toward the surface implies that in equilibrium, electron cannot move to surface from the bulk.
3. All bands bend up by the same amount, indicating that both the bandgap and electron affinity are not affected by surface states.
Workfunction measurement

1. Photoemission
   consider a metal surface illuminated by monoenergetic photons of energy $hv$ greater than the work function of the metal surface.

Work function = $hv$ – energy width of the photoelectron spectrum

The accuracy is determined by the ability to locate the start of secondary electron background and Fermi edge and is about 0.1eV
2. Kelvin Method

The Kelvin method is used to measure work function changes relative to a reference probe surface that has a stable work function value.

\[ I(=dQ/dt) = (V + V_{ext})dC/dt \]

If \( V_{ext} = -\Delta V \), \( I = 0 \). This gives the work function relative to the reference probe surface.

The accuracy is 1-10 Mev
Workfunction measurement

3. Retarding field technique
   A beam of monoenergetic electrons impinges on the specimen surface, the current flowing into the specimen is measured as a function of the retarding voltage applied to the specimen.

   Current vanishes when vacuum level of the specimen is just above that of filament. If the work function of the specimen changes, the amount of retarding voltage will be changed.

   Work function change = the difference in the retarding voltage.

   The accuracy is 10 – 100 Mev
Now consider a metal/n type semiconductor interface, with the work function of the metal greater than that of the semiconductor.

The metal-semiconductor interface

a. Charge distribution

b. Energy band diagram according to the Schottky model \((\phi_M > \phi_{sc})\)
Metal

Semiconductor

In a steady state

\[ J_{th,m} + J_r = J_{th,s} \]

Then, we get the net electron current flow \( J(-V) \) from the semiconductor to the metal when a voltage \(-V\) is applied to the semiconductor

\[ J(-V) = J_{th,s} \left[ \exp \left( \frac{eV}{k_B T} \right) - 1 \right] \]
The asymmetry in charge transport across the interface is nonohmic behavior. The particular system is called a Schottky diode. More treatment shows $J_{th,s}$ to be proportional to $\sqrt{V_{BB} - V}$. Then, we can get

$$J(-V) = J_0 \left[ \exp \left( \frac{eV}{nk_B T} \right) - 1 \right]$$

Where $n$ is the ideality factor. This equation is valid only when $V \ll V_{BB}$. and $n \approx 1 + (k_B T/2eV_{BB})$. 
Discussion: The electrical properties of a metal/N type semiconductor interface when the work function of the metal is less than that of the semiconductor using the Schottky model.

In this case, the semiconductor bands bend downward at the interface. This implies that the conduction band at the interface is closer to the Fermi level than in the bulk. Since the conduction electron concentration in a semiconductor is proportional to, this means that there is a higher conduction electron concentration at the interface. Therefore, the interface is no longer a region that limits the conductance of the metal semiconductor system. Under these conditions, the metal semiconductor junction is ohmic.
Thank you!