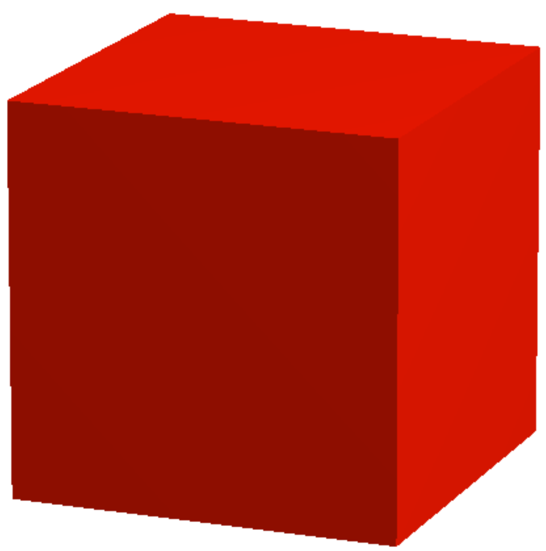
Finite solids / nano-structures

- Small is different:
  - quantum confinement
  - high relative surface area
- Magnetism in nano-structures
- Interesting new physics in two and one dimensions

Small is different

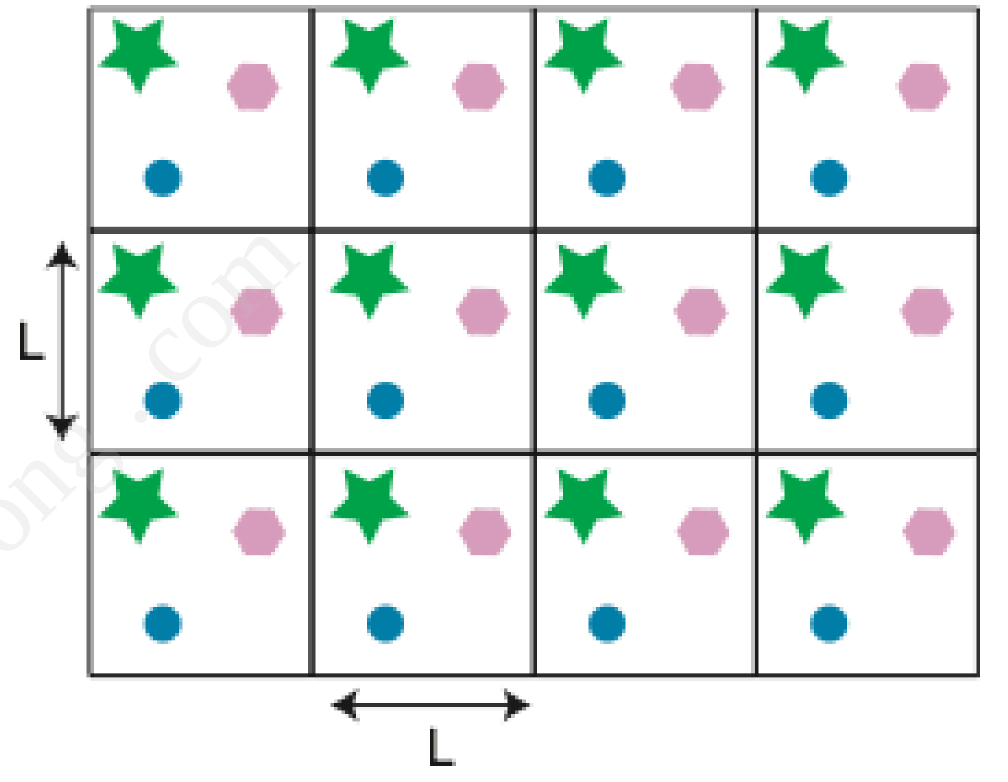


change of bulk properties

increased importance of surfaces

Periodic boundary conditions

Max Born and Theodore von Karman (1912)



- We want to get rid of the surface restrictions, i.e. we want a solid which is finite in size but has no surfaces (!).
- If we move by one crystal size L, we have to get the same.

$$u(x, y, z) = u(x + L, y + L, z + L)$$

The surface was invented by the devil - Wolfgang Pauli

Periodic boundary conditions

chain with lattice spacing *a* and macroscopic side length *L=Na*:

1D

$$k = \frac{2\pi}{aN} n$$

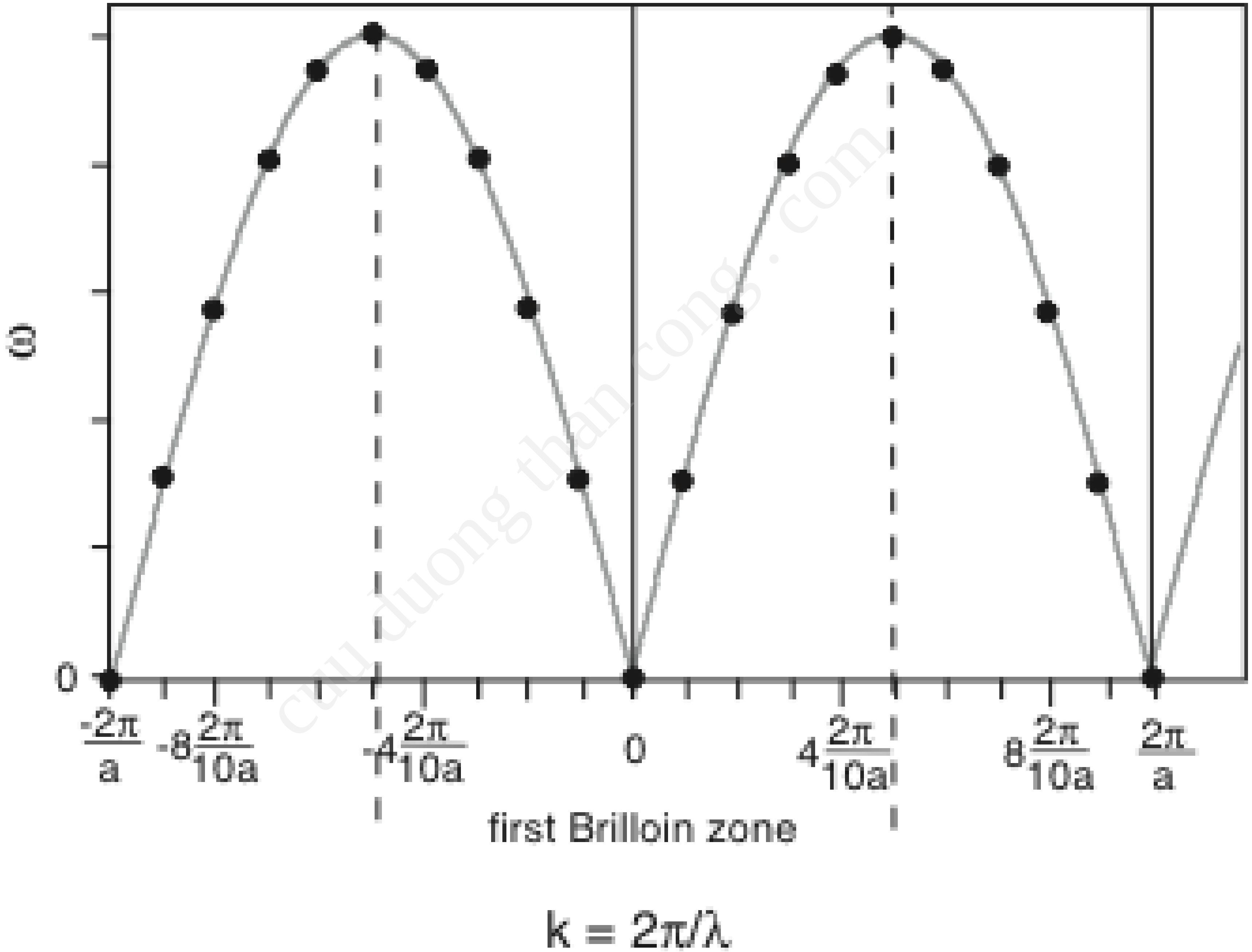
cubic crystal with lattice spacing *a* and macroscopic side length *L=na*:

3D

$$\mathbf{k} = (k_x, k_y, k_z) = \frac{2\pi}{aN}(n_x, n_y, n_z) = (\frac{n_x 2\pi}{L}, \frac{n_y 2\pi}{L} \frac{n_z 2\pi}{L})$$

Finite chain with 10 unit cells and one atom per unit cell

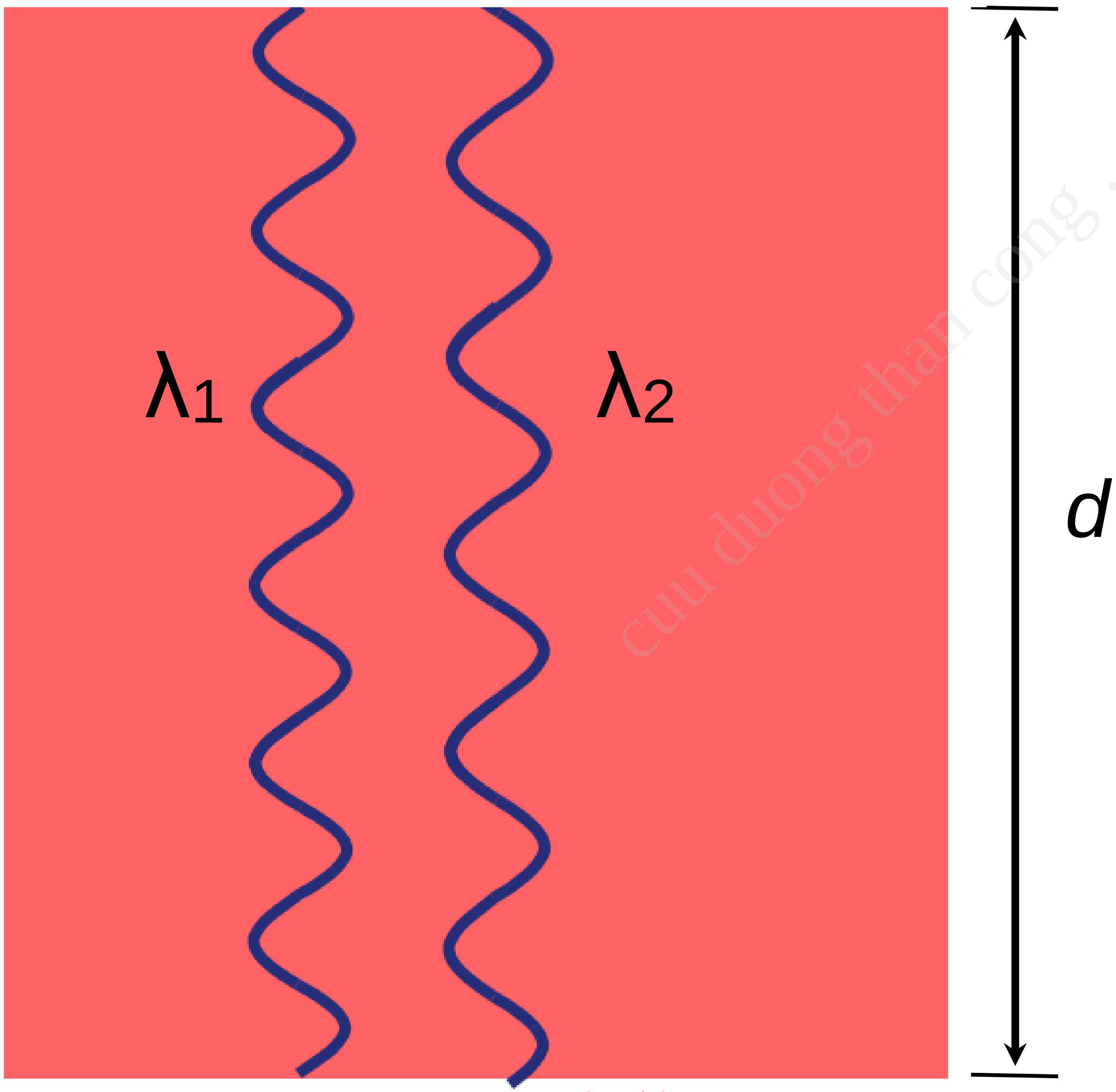
$$k = \frac{2\pi}{aN} n$$



- N atoms give N so-called normal modes of vibration.
- For long but finite chains, the points are very dense.

Quantum-size effects

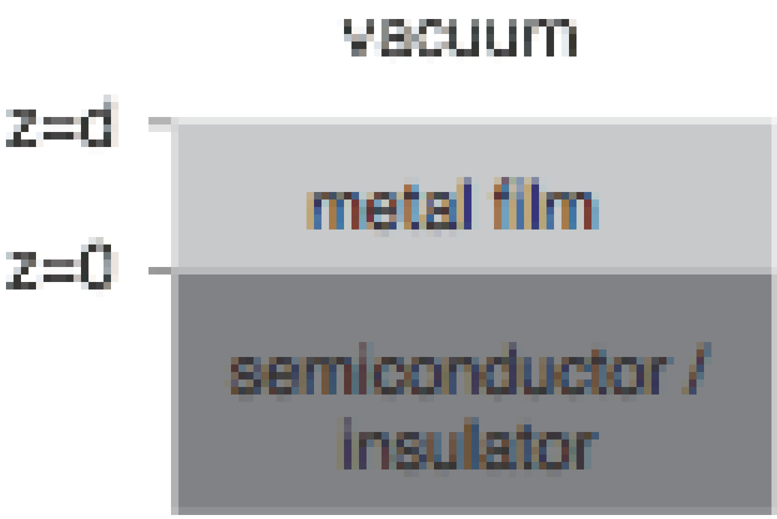
thick film
(particle in a potential well)

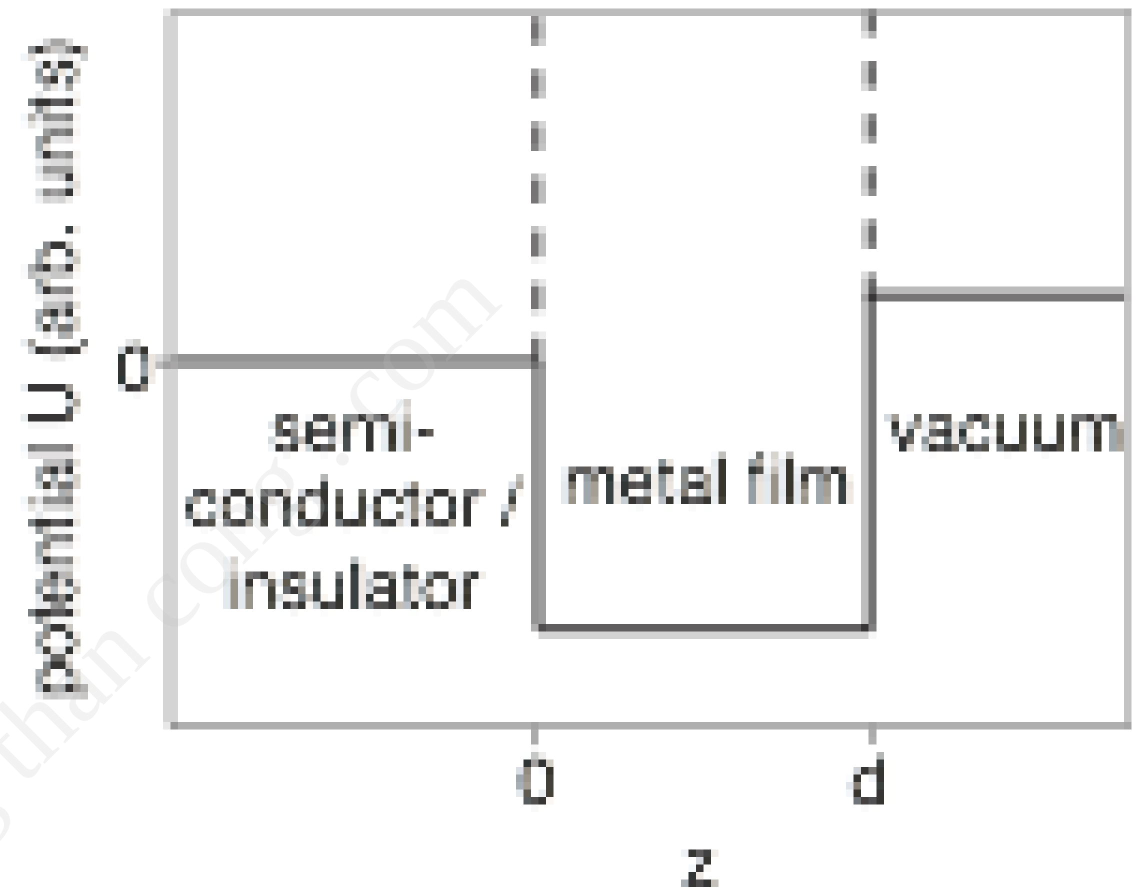


$$k = \frac{2\pi}{\lambda}$$

$$E = \frac{\hbar^2 k^2}{2m^*}$$

Quantum size effects



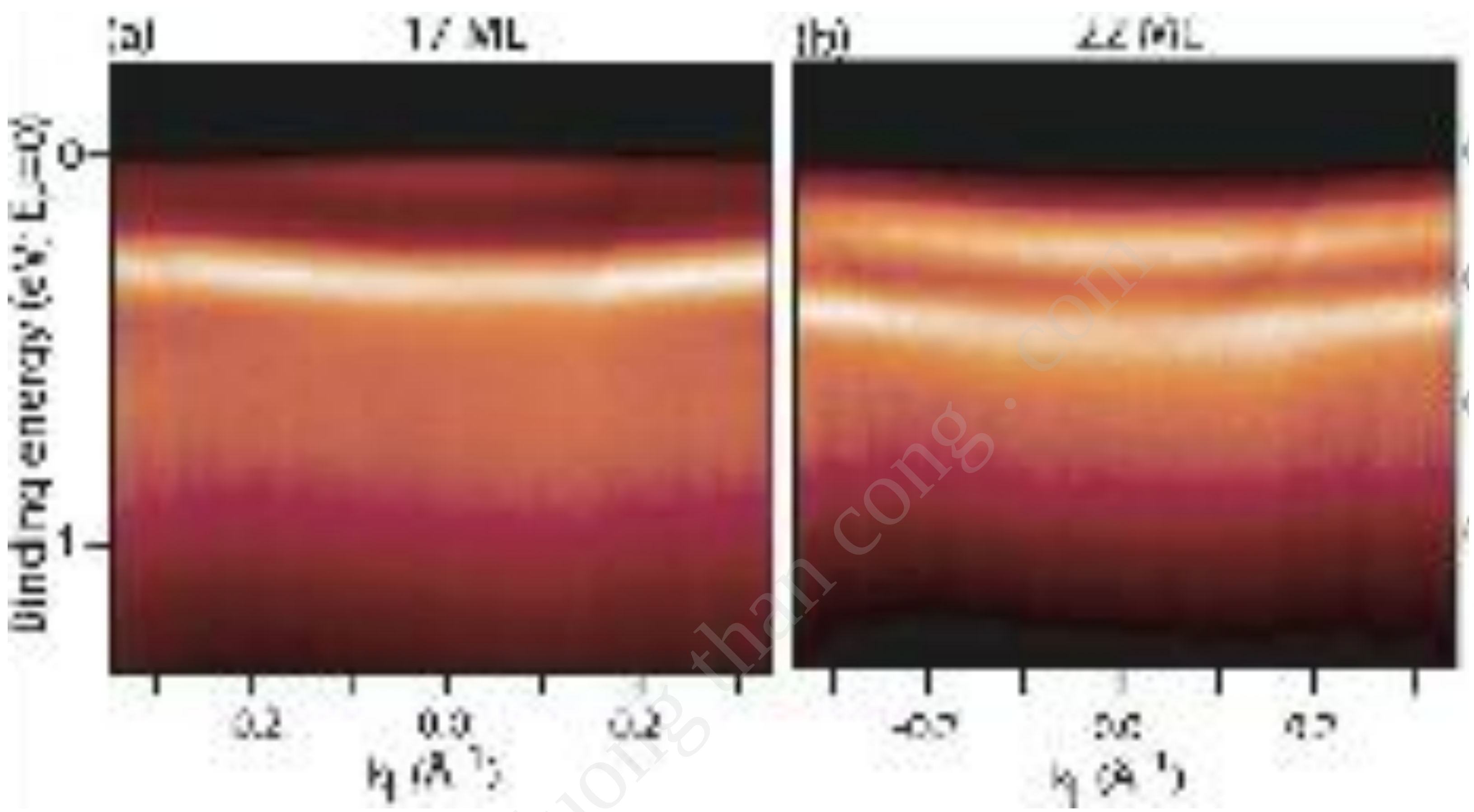


$$\Psi(\mathbf{r}) = \Psi(z)\Psi(x,y)$$

$$E_{xy} = \frac{\hbar^2 \mathbf{k}_{xy}^2}{2m_e}$$

$$\Psi(z) = Ae^{ik_z z} + Be^{-ik_z z}$$

Thin films: free electrons in the other direction

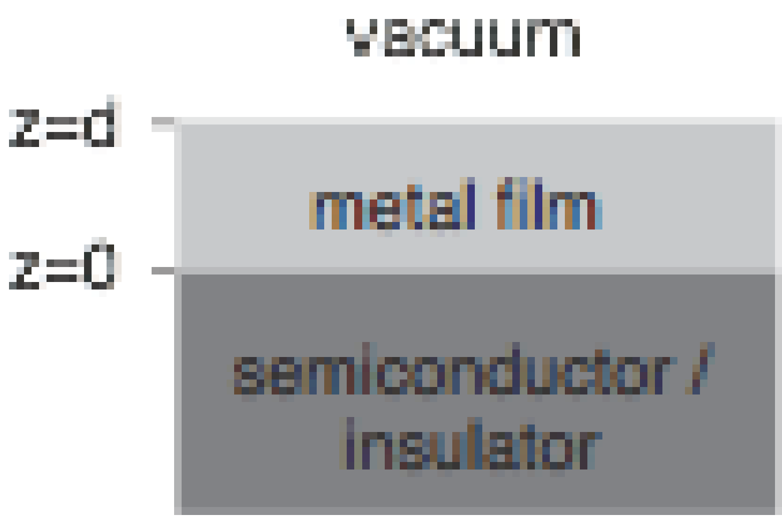


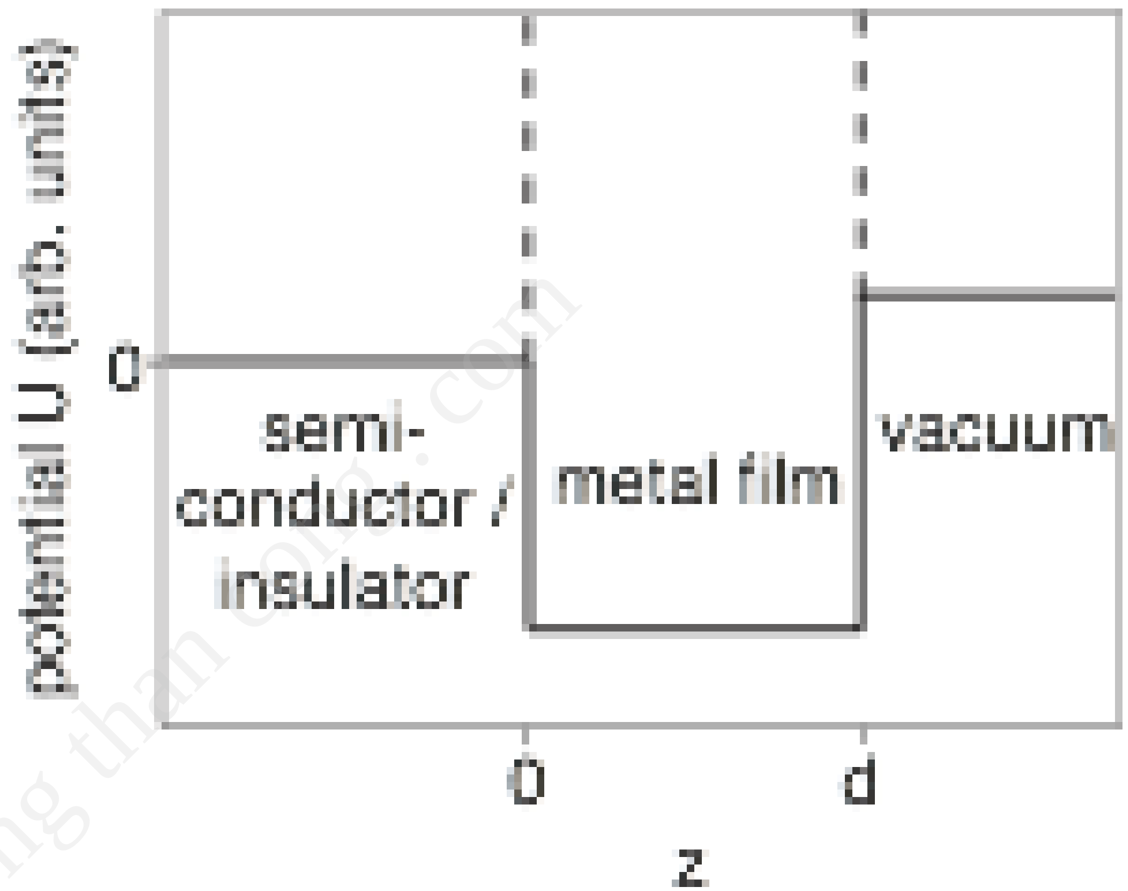
$$\Psi(\mathbf{r}) = \Psi(z)\Psi(x, y)$$

$$E_{xy} = \frac{\hbar^2 \mathbf{k}_{xy}^2}{2m_e} \qquad \Psi(z) = Ae^{ik_z z} + Be^{-ik_z z}$$

- parabolic dispersion parallel to the film
- quantization in film direction

Quantum size effects





for an infinite well, the wave function has to vanish at the boundaries

$$2d = n\lambda.$$

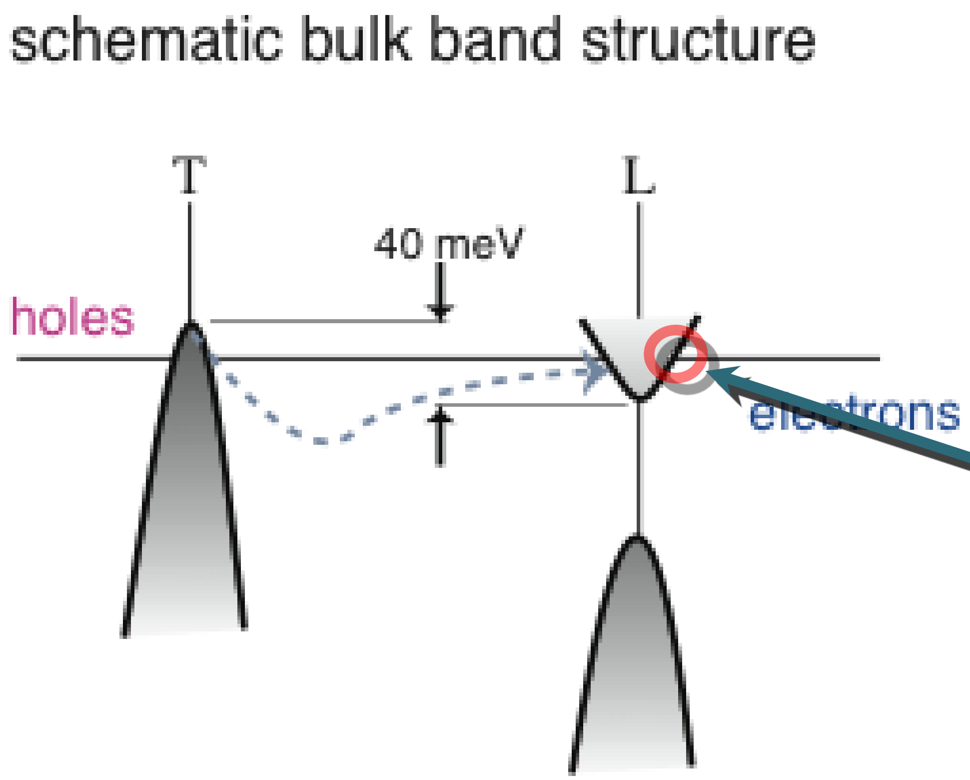
$$2k_z d = n2\pi \qquad n = 1, 2, 3...$$

$$E_z = \frac{\hbar^2 k_z^2}{2m_e}$$

for a finite well

$$2k_z d + \Phi_i + \Phi_v = 2\pi n \qquad n = 1, 2, 3...$$

Quantum size effects in thin Bi films



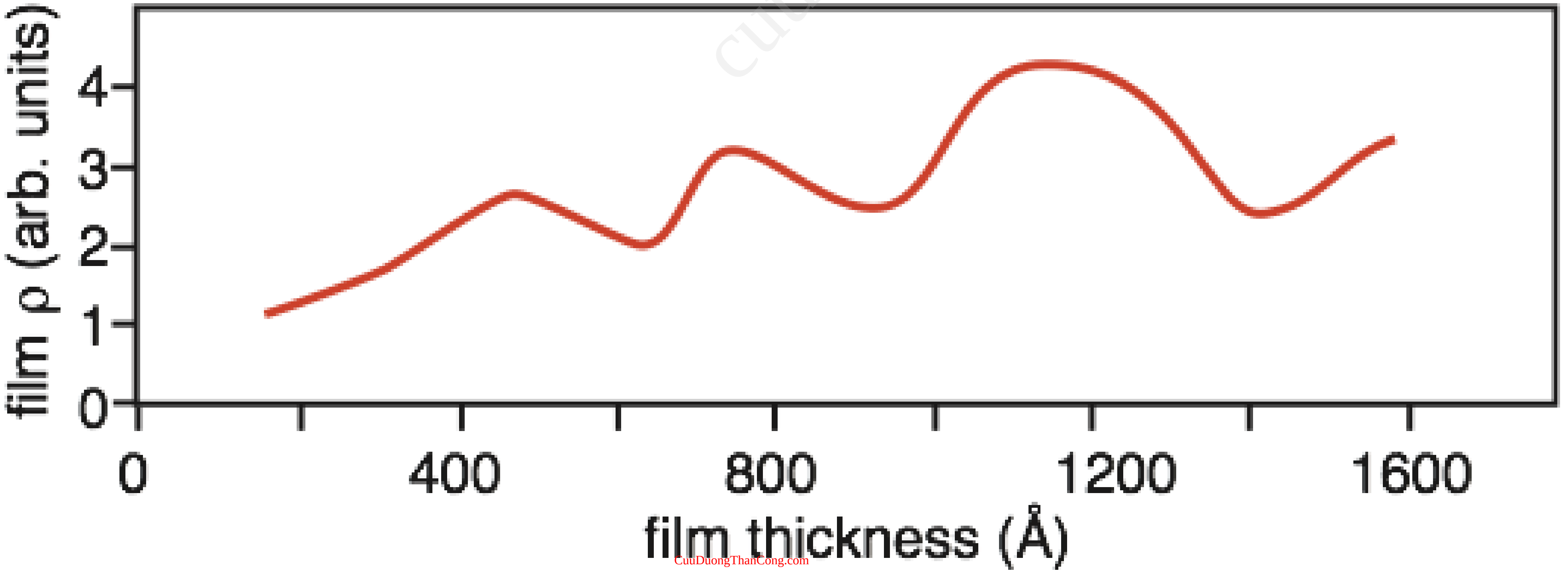
small

$$E(k) = -E_0 + \frac{\hbar^2 k^2}{2m^*}$$

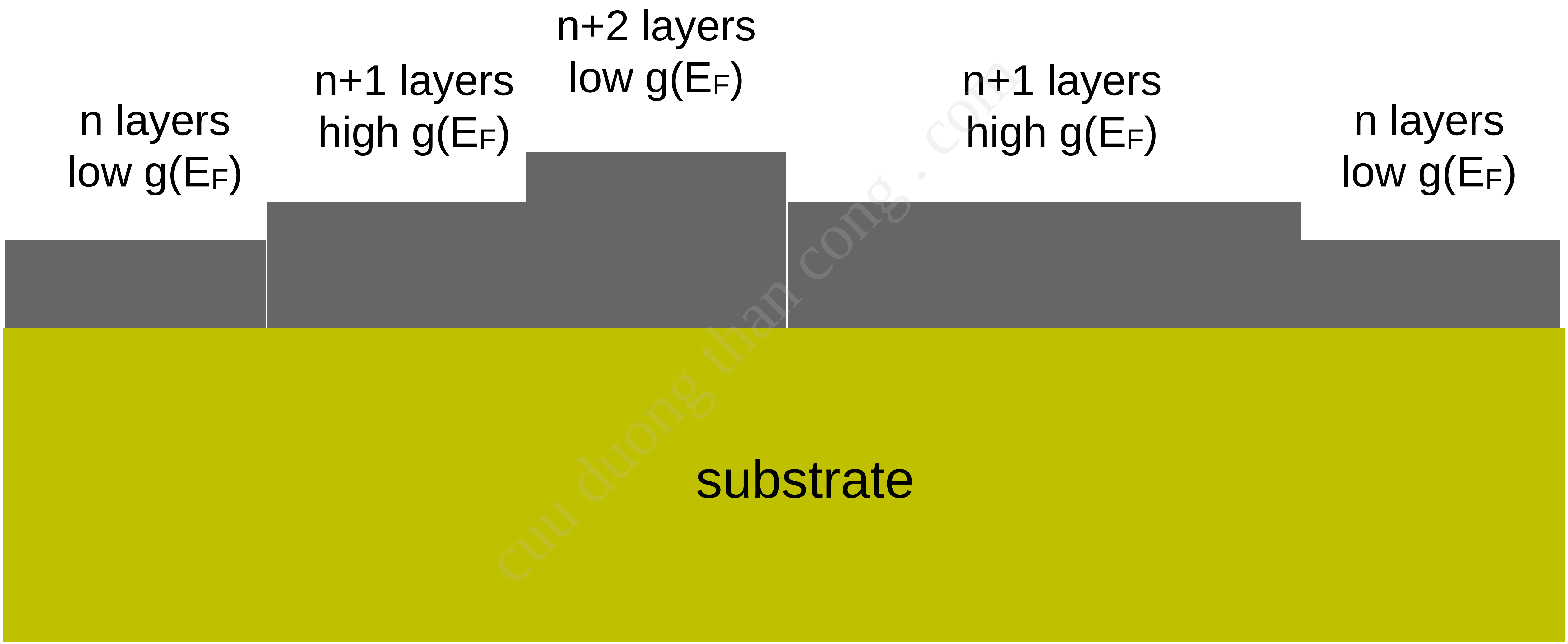
small

k_F very small

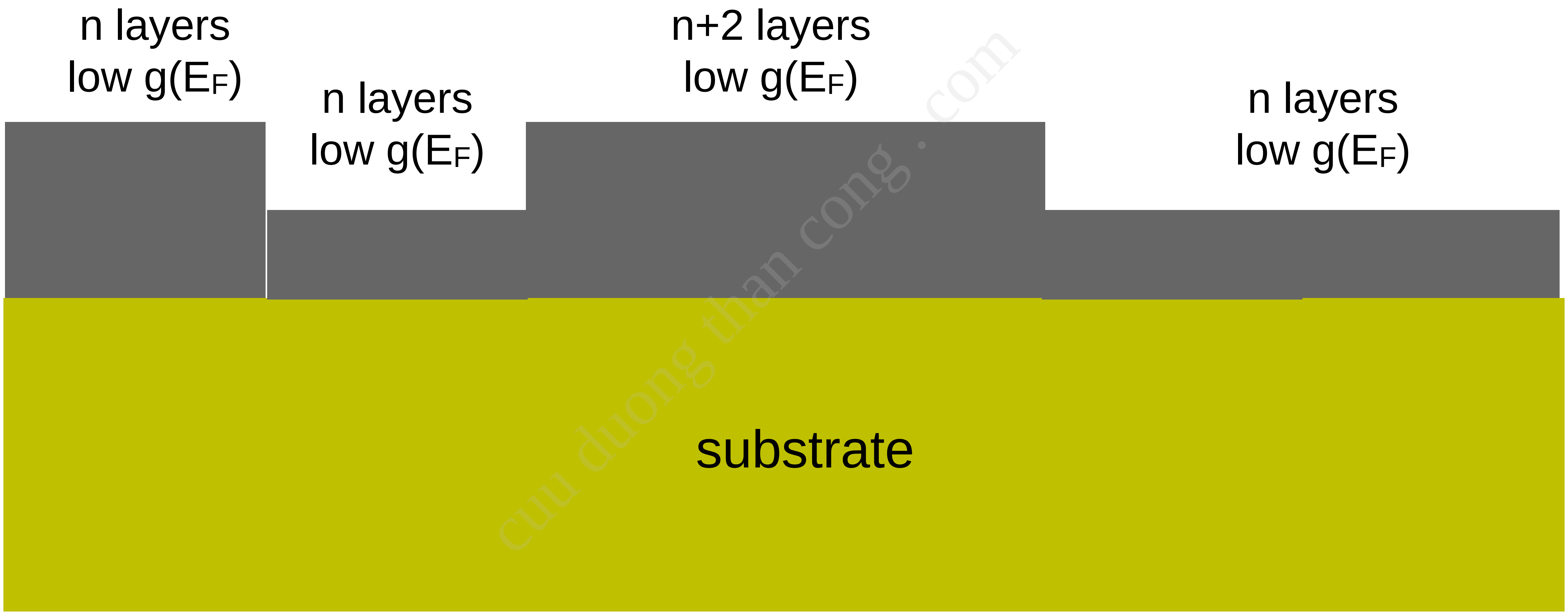
λ_F very long (hundreds of Å)



Magic film height



Magic film height



Semiconductor nanoparticles

bulk semiconductors: smallest energy to create e-h pair

$$E_{\min} = E_g$$

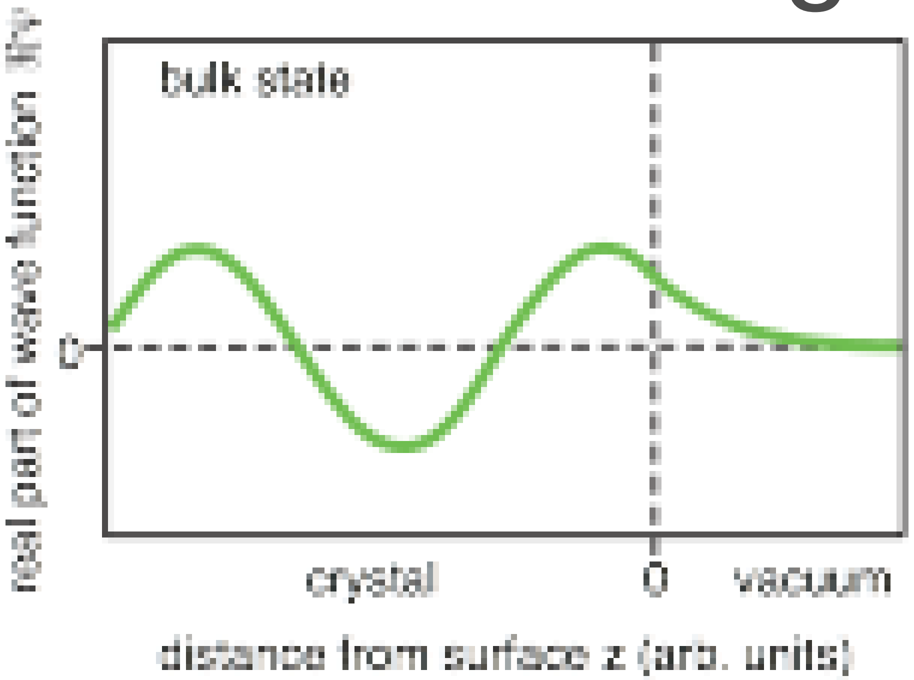
semiconductor nano-crystal

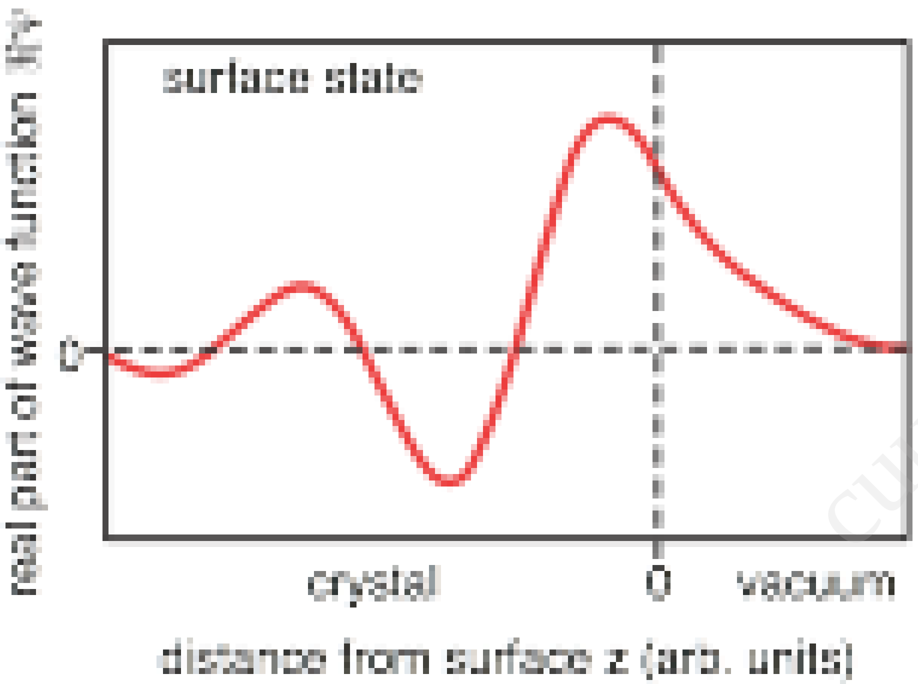
$$E_{\min} = E_g + \frac{\hbar^2 \pi^2}{2 \mu r^2} - \frac{1.8 e^2}{4 \pi \epsilon_0 \epsilon r}$$

quantum confinement

Coulomb interaction

New genuine surface states





$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$

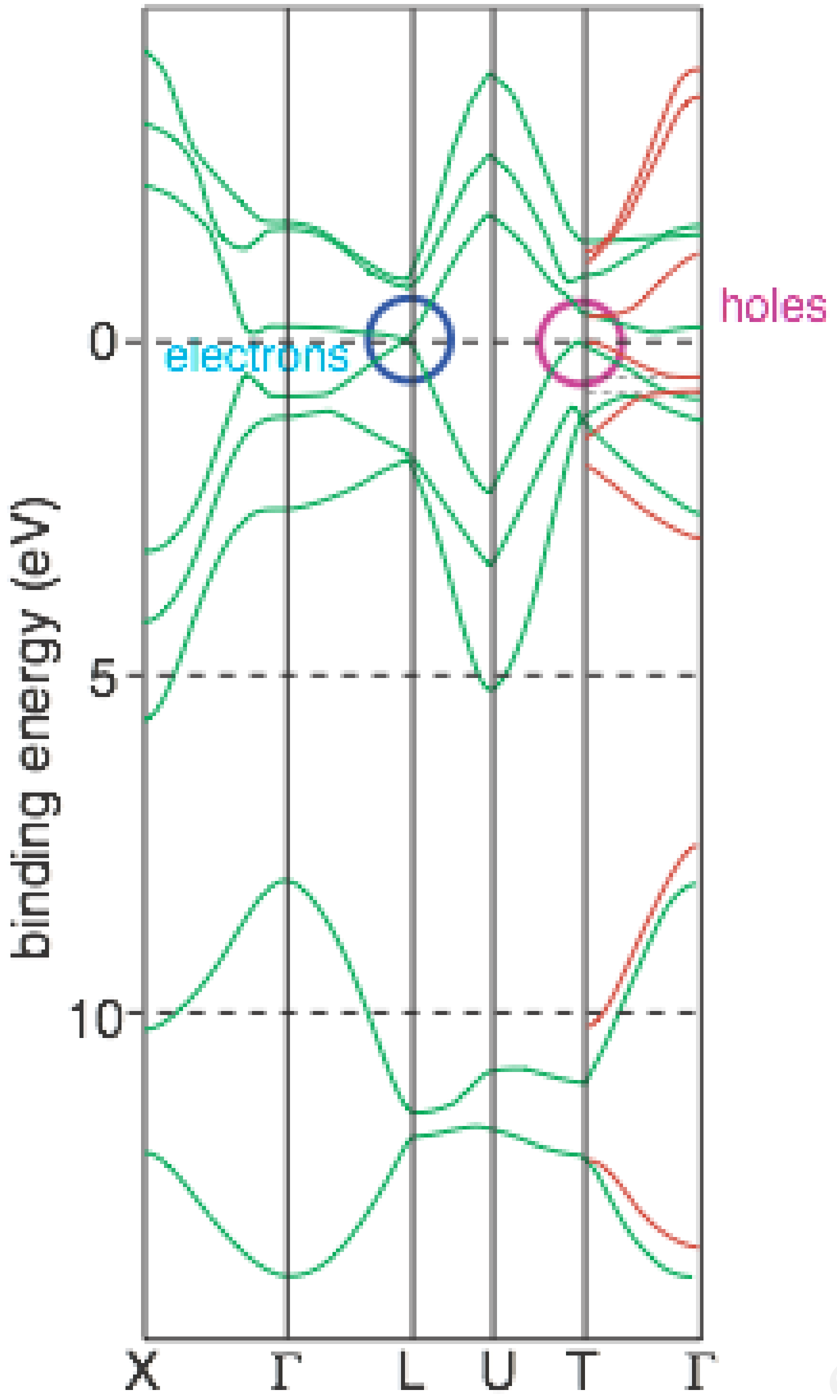
if k was complex

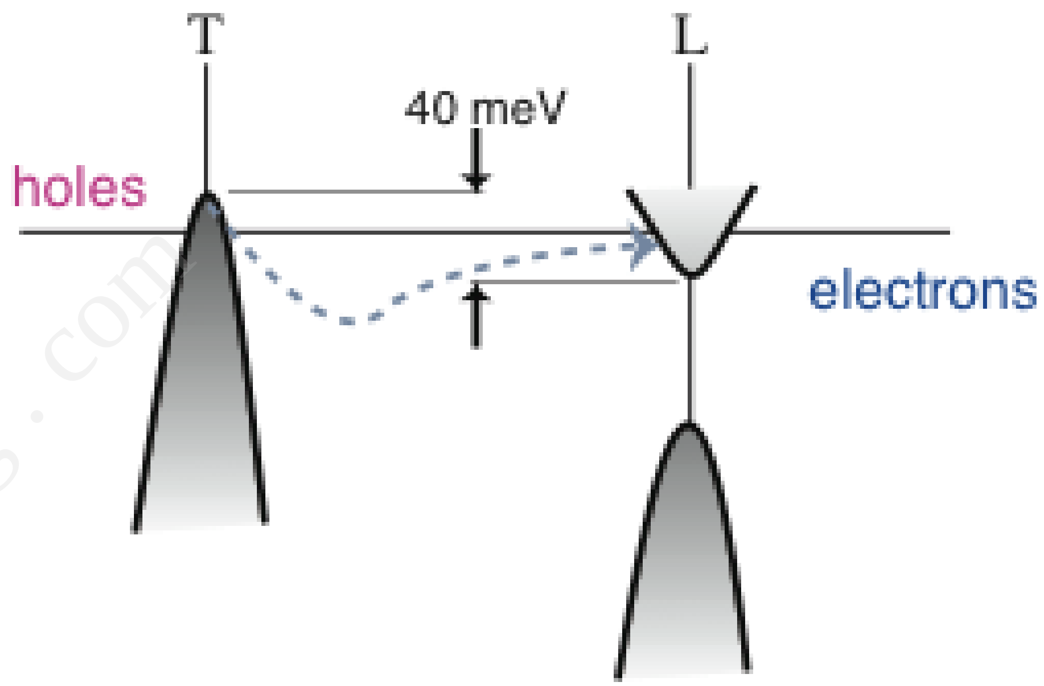
$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{\Im(k_z)z} e^{i\mathbf{k}'\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$

at the surfaces

$$\psi_{\mathbf{k}_{||}}(\mathbf{r}) = e^{i\mathbf{k}_{||}\cdot\mathbf{r}_{||}} u_{\mathbf{k}_{||}}(\mathbf{r}_{||}) e^{i\kappa z}$$

Electronic structure of Bi



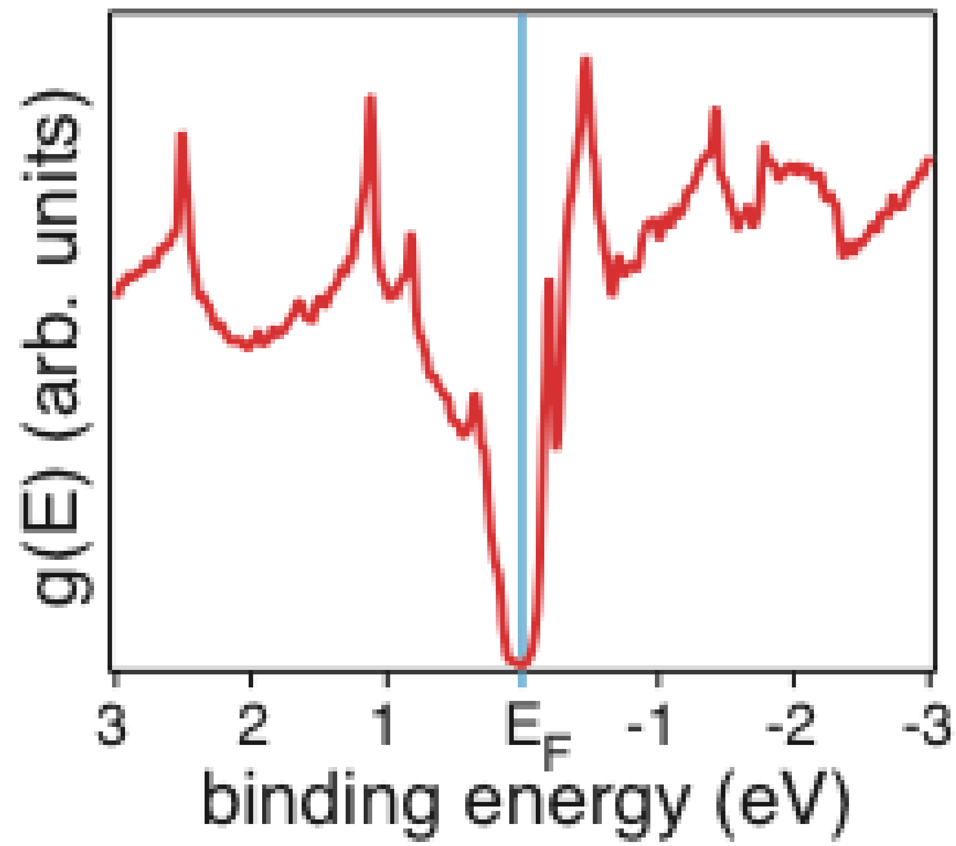


$$T_C = 1.13\Theta_D \exp \frac{-1}{g(E_F)V}$$

Debye temp.

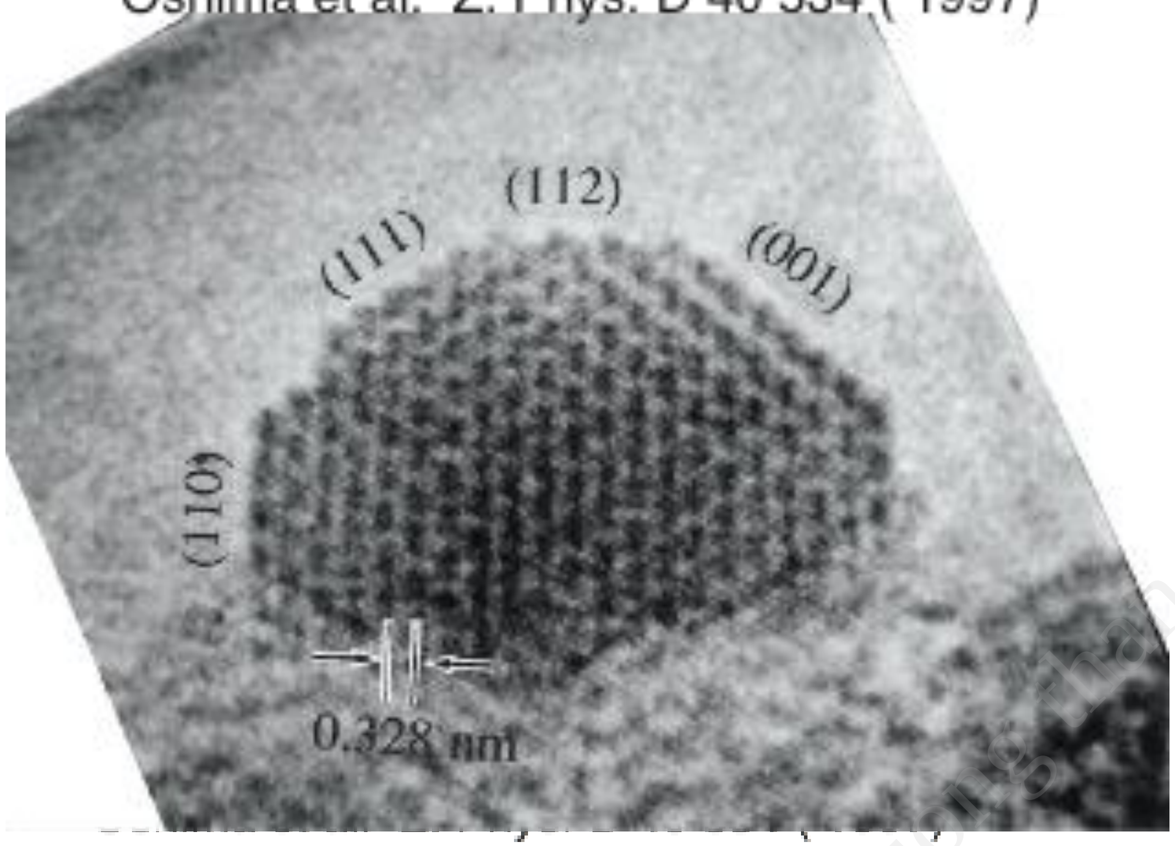
density of states

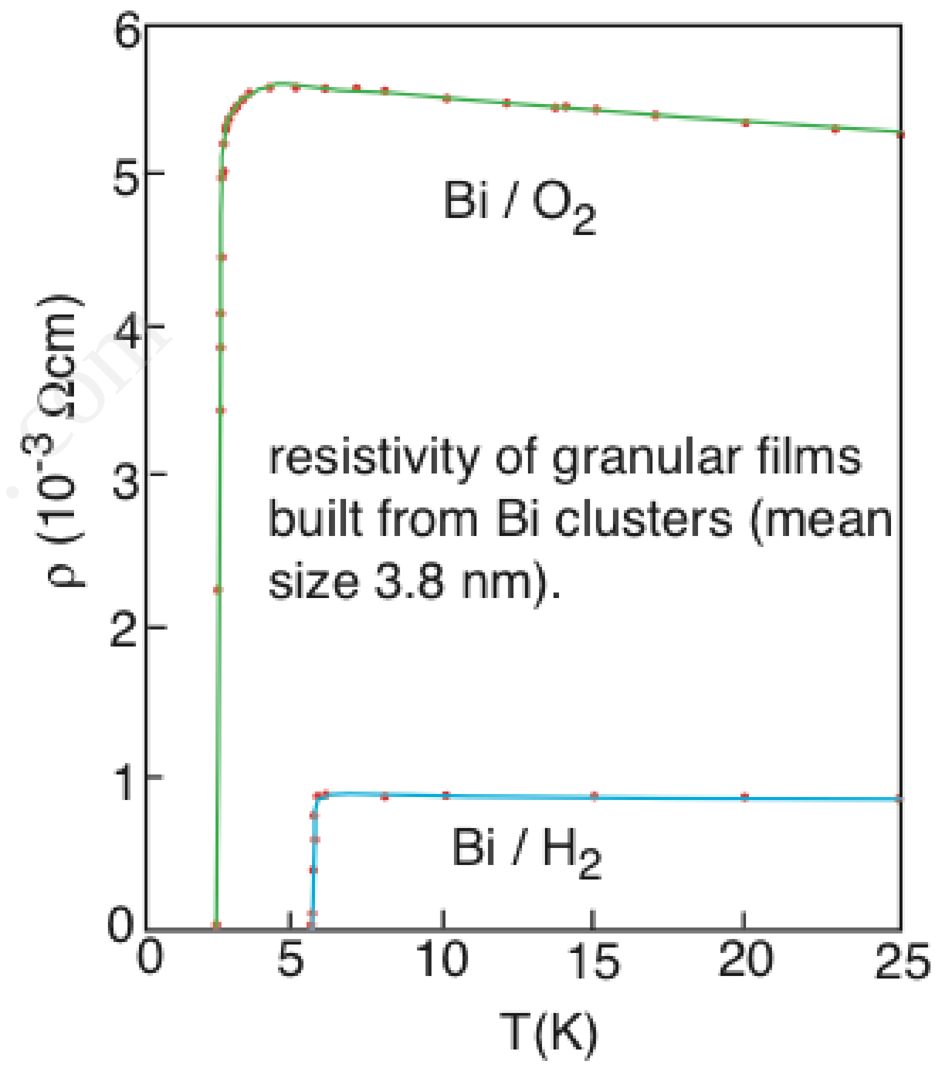
el-ph interaction strength



Superconductivity in Bi nanoclusters

Oshima et al. Z. Phys. D 40 534 (1997)





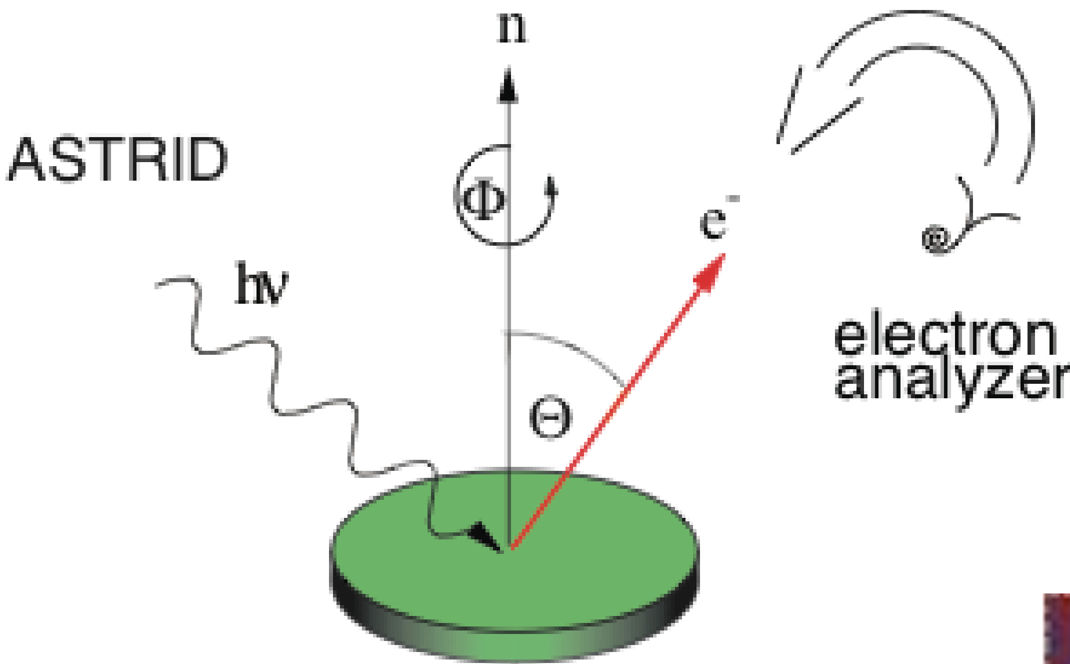
Weitzel and Micklitz, PRL **66**, 385 (1991)

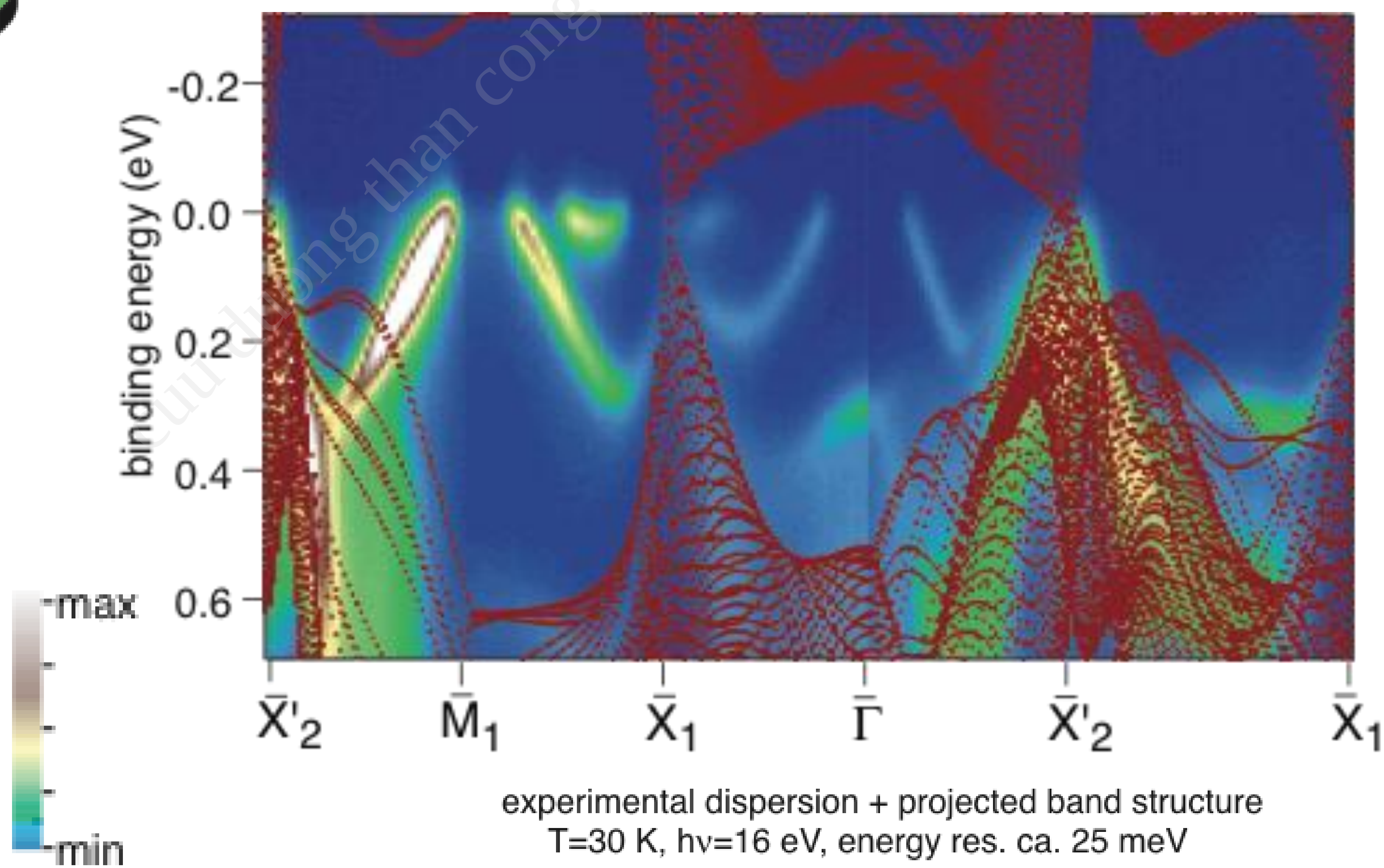
- Bulk Bi is not superconducting.
- Granular films of Bi clusters are superconducting at several K.
- T_c is increasing for decreasing cluster size.
- T_c depends on the environment.

Superconductivity caused by metallic surface?

$$T_c = 1.13\Theta_D \exp\left[\frac{-1}{N(E_F)V}\right]$$

Electronic structure of Bi(110)

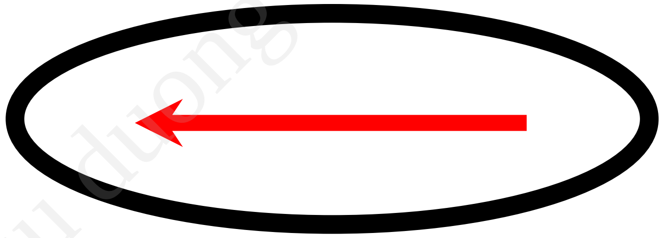




experimental dispersion + projected band structure
T=30 K, hν=16 eV, energy res. ca. 25 meV

Superparamagnetism

- Bulk magnet: flipping one spin costs energy ≈ $k_B\theta_C$.
- Nano-magnet: all the spins in the single domain can be rotated at the same time. This costs much less energy.



$$\Delta E \approx VMB_{\text{inside}} \approx V\mu_0 M^2$$