

第三章 简单体系的薛定谔方程(12学时)

- 3.1 自由电子及平面波
- 3.2 量子阱、量子线与量子点
- 3.3 谐振子与氢原子简介

3.1 自由电子及平面波

1. 自由粒子定态薛定谔方程的解

- ① 解薛定谔方程的一般方法及定态薛定谔方程的含义
- ② 自由粒子定态薛定谔方程的平面波解：一维，三维
- ③ 平面波的时间依赖关系与自由粒子波函数的演化
- ④ 通过对易关系找定态薛定谔方程的解

2. 守恒力学量

- ① 动量的期望值及其随时间的依赖关系：用general公式推导；用测量几率密度的含义推导
- ② 与哈密顿算符对易的力学量是守恒量：直接推导；共同本征函数推导

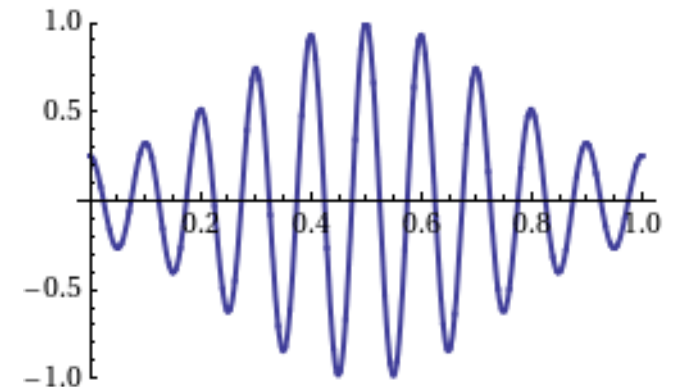
3.1 自由电子及平面波

3. 平面波的色散关系

- ① 一维情况的色散关系
- ② 相速度

4. 波包与群速度

- ① 波包
- ② 群速度是包络的运动速度，相速度是载波的运动速度
- ③ 自由电子的运动速度：群速度



3.1 自由电子及平面波

5. 有限空间中的平面波

① 周期边界条件：当电子运动范围很大时，边界条件的选取对大多数结论不重要，所以可以选择周期性边界条件（Born-Von Karman boundary condition）

② 一维情况

$$\psi(x=0) = \psi(x=L), \text{ 从而 } k_n = \frac{2\pi}{L}n, \quad E_n = \frac{\hbar^2 k_n^2}{2m}, \quad n \text{ 取值所有整数}$$

③ 三维情况

$$\mathbf{k}_{m,n,l} = \left(\frac{2\pi}{L_x}m, \frac{2\pi}{L_y}n, \frac{2\pi}{L_z}l \right), \quad E_n = \frac{\hbar^2 |\mathbf{k}_{m,n,l}|^2}{2m}, \quad (m,n,l) \text{ 取值所有整数}$$

3.1 自由电子及平面波

6. 泡利不相容原理

每个独立的量子状态只能被一个电子占据
内禀的量子关联，与库伦相互作用等无关

7. 自由电子气的费米能和费米波矢

$$E_F = \frac{\hbar^2 k_F^2}{2m_e}$$

3.1 自由电子及平面波

7. 自由电子气的费米能和费米波矢

$$1\text{D}: k_F = \frac{1}{2}\pi n$$

$$2\text{D}: k_F = \sqrt{2\pi n}$$

$$3\text{D}: k_F = (3\pi^2 n)^{1/3}$$

8. 自由电子气的态密度(DOS)

$$1\text{D}: D(E) = \frac{1}{\pi\hbar} \sqrt{\frac{2m}{E}}$$

$$2\text{D}: D(E) = \frac{m}{\pi\hbar^2}$$

$$3\text{D}: D(E) = \frac{m}{\pi^2\hbar^3} \sqrt{2mE}$$

3.2 量子阱、量子线与量子点

1. 一维无限深势阱问题

$$V(x) = \begin{cases} 0 & 0 \leq x \leq W \\ \infty & otherwise \end{cases}$$

$$\psi_n(x) = \sin(k_n x), \quad k_n = \frac{\pi}{W} n, \quad E_n = \frac{\hbar^2 k_n^2}{2m_e} = \frac{\hbar^2 \pi^2}{2m_e W^2} n^2, \quad n \text{取值所}$$

有正整数

驻波: $\psi_n(x, t) = \sin(k_n x) \exp(-iE_n t/\hbar)$

零点能: 动量为零要求位置无限扩展

3.2 量子阱、量子线与量子点

2. 量子阱

① x方向受限, yz方向 “自由”

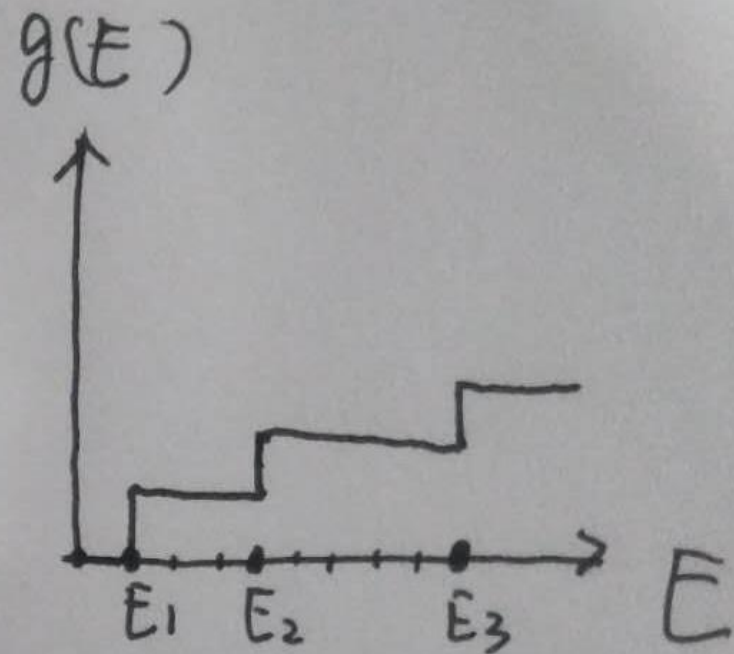
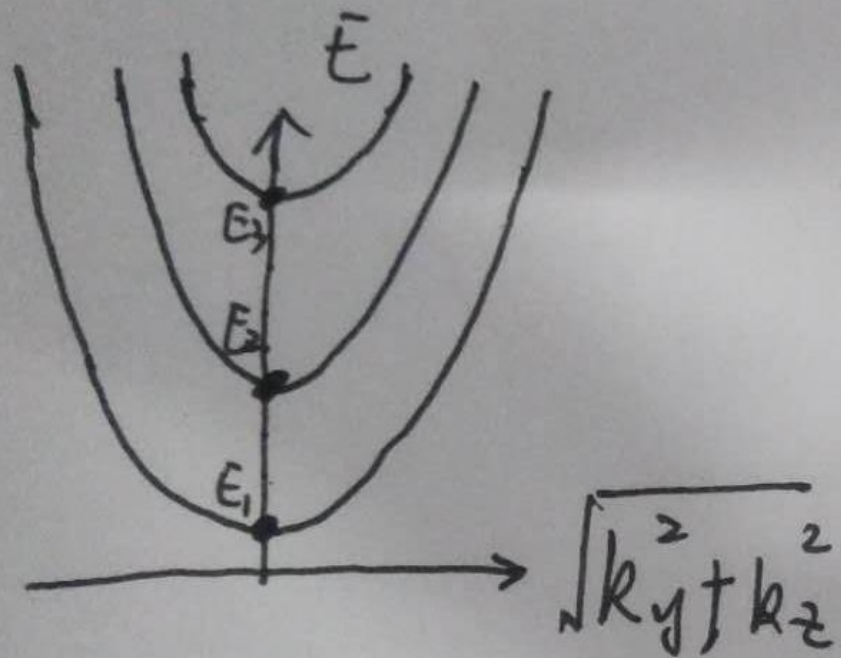
$$\psi_{n,k_y,k_z}(\mathbf{r}) = \sin\left(\frac{n\pi}{W}x\right) \exp(ik_y y) \exp(ik_z z), \quad E_{n,k_y,k_z} = \frac{\hbar^2 \pi^2}{2m_e W^2} n^2 + \frac{\hbar^2 (k_y^2 + k_z^2)}{2m_e}, \quad n \text{ 取值所有正整数}$$

② 能带的概念

3.2 量子阱、量子线与量子点

2. 量子阱

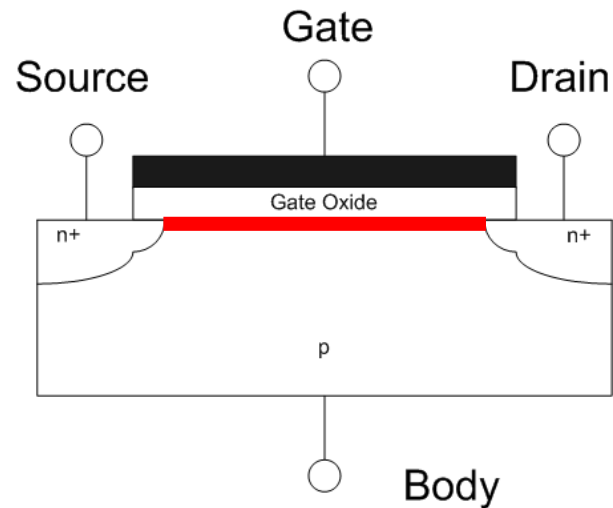
- ③ 二维自由电子气（第一个能带）： $k_F = (2\pi n)^{1/2}$, $E_F = \hbar^2 k_F^2 / 2m_e$, $D(E) = \frac{m_e}{\hbar^2 \pi}$
- ④ 考虑多个能带的情况



3.2 量子阱、量子线与量子点

2. 量子阱

⑤ 实际体系一：MOSFET



New Method for High-Accuracy Determination of the Fine-Structure Constant Based on Quantized Hall Resistance

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(Received 30 May 1980)

Measurements of the Hall voltage of a two-dimensional electron gas, realized with a silicon metal-oxide-semiconductor field-effect transistor, show that the Hall resistance at particular, experimentally well-defined surface carrier concentrations has fixed values which depend only on the fine-structure constant and speed of light, and is insensitive to the geometry of the device. Preliminary data are reported.

PACS numbers: 73.25.+i, 06.20.Jr, 72.20.My, 73.40.Qv

In this paper we report a new, potentially high-accuracy method for determining the fine-structure constant, α . The new approach is based on the fact that the degenerate electron gas in the inversion layer of a MOSFET (metal-oxide-semiconductor field-effect transistor) is fully quantized when the transistor is operated at helium temperatures and in a strong magnetic field of order 15 T.¹ The inset in Fig. 1 shows a schematic diagram of a typical MOSFET device used in this work. The electric field perpendicular to the surface (gate field) produces subbands for the motion normal to the semiconductor-oxide interface, and the magnetic field produces Landau quantization of motion parallel to the interface. The density of states $D(E)$ consists of broadened δ functions²; minimal overlap is achieved if the magnetic field is sufficiently high. The number of states, N_L , within each Landau level is given by

$$N_L = eB/h, \quad (1)$$

where we exclude the spin and valley degeneracies. If the density of states at the Fermi energy, $N(E_F)$, is zero, an inversion layer carrier cannot be scattered, and the center of the cyclotron orbit drifts in the direction perpendicular to the electric and magnetic field. If $N(E_F)$ is finite but small, an arbitrarily small rate of scattering cannot occur and localization produced by the long lifetime is the same as a zero scattering rate, i.e., the same absence of current-carrying states occurs.³ Thus, when the Fermi level is between

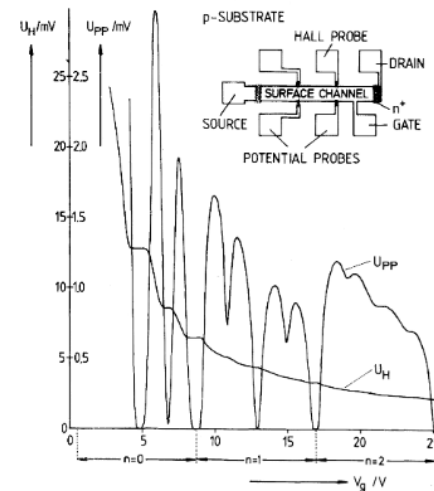
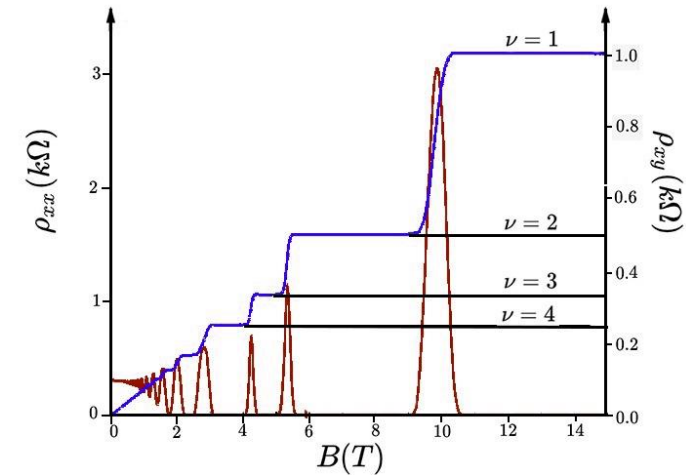


FIG. 1. Recordings of the Hall voltage U_H , and the voltage drop between the potential probes, U_{PP} , as a function of the gate voltage V_g at $T=1.5$ K. The constant magnetic field (B) is 18 T and the source drain current, I , is 1 μ A. The inset shows a top view of the device with a length of $L=400$ μ m, a width of $W=50$ μ m, and a distance between the potential probes of $L_{PP}=130$ μ m.

量子效应显现的条件：
低缺陷、低温



The Nobel Prize in Physics 1985



Photo from the Nobel Foundation archive.

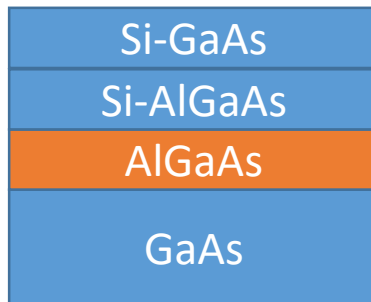
Klaus von Klitzing

Prize share: 1/1

3.2 量子阱、量子线与量子点

2. 量子阱

⑥ 实际体系二：AlGaAs异质结



The Nobel Prize in Physics 1998



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Robert B. Laughlin

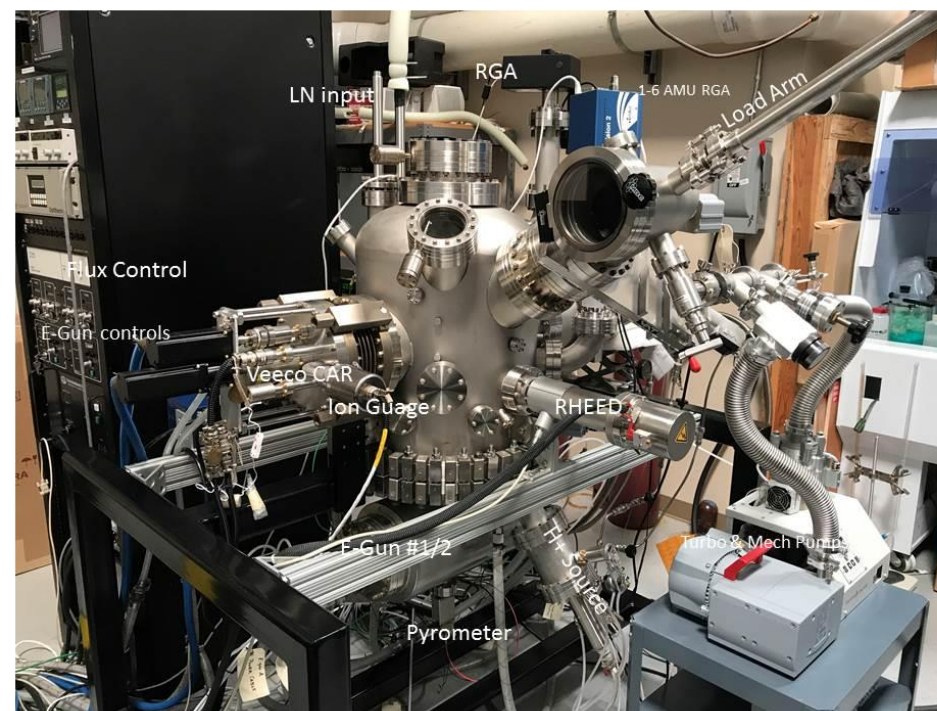
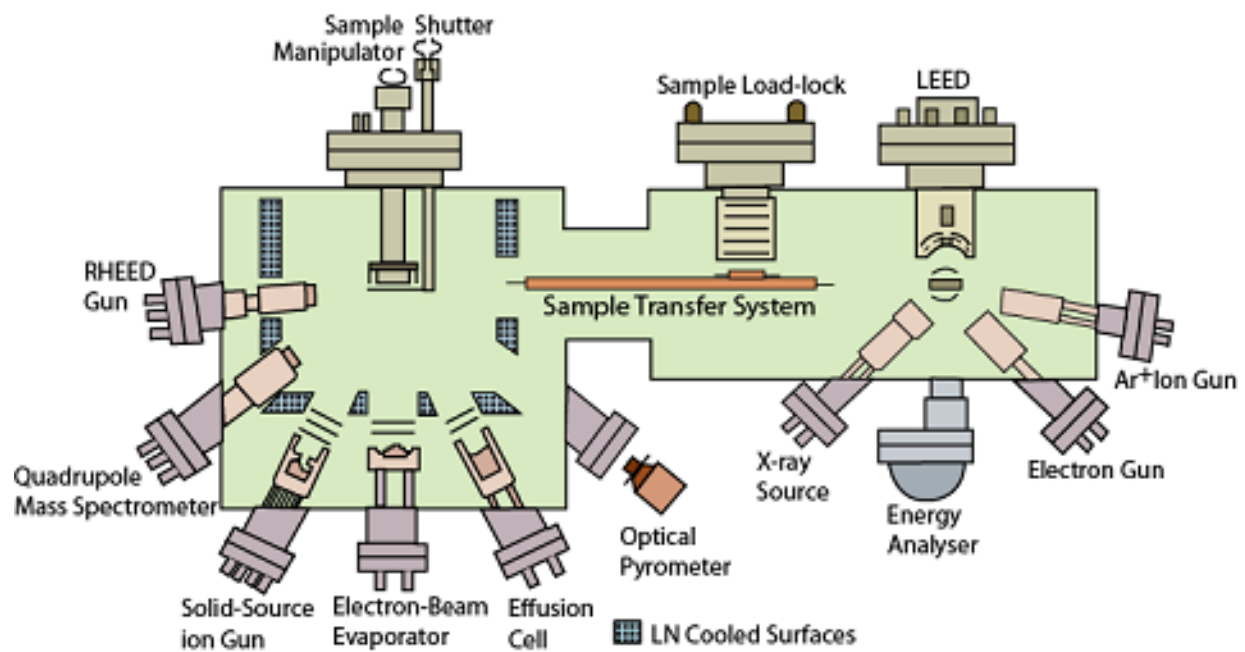


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分数量子霍尔效应, 1982

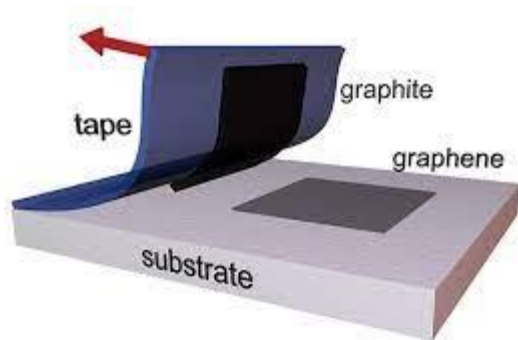
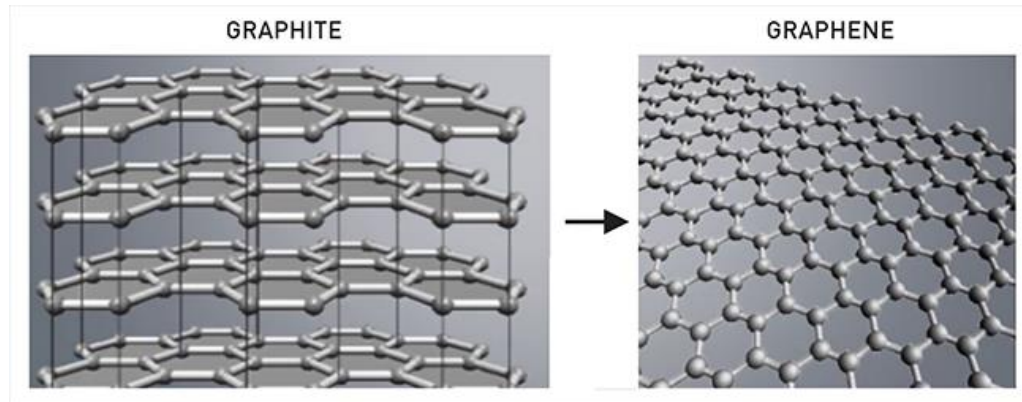


分子束外延

3.2 量子阱、量子线与量子点

2. 量子阱

⑦ 实际体系三：二维材料



The Nobel Prize in Physics 2010



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Andre Geim

Prize share: 1/2



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Konstantin Novoselov

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3.2 量子阱、量子线与量子点

3. 量子线

① xy方向受限, z方向 “自由”

$$\psi_{m,n,k_z}(\mathbf{r}) = \sin\left(\frac{m\pi}{W_x}x\right) \sin\left(\frac{n\pi}{W_y}y\right) \exp(ik_z z),$$

$$E_{m,n,k_z} = \frac{\hbar^2 \pi^2}{2m_e W_x^2} m^2 + \frac{\hbar^2 \pi^2}{2m_e W_y^2} n^2 + \frac{\hbar^2 k_z^2}{2m_e}, \quad m, n \text{ 取值所有正整数}$$

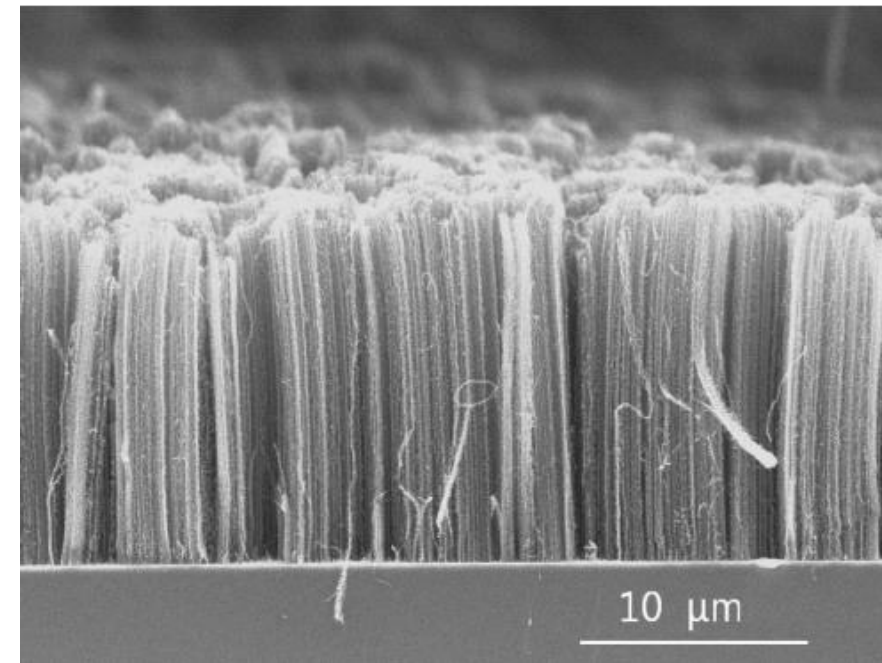
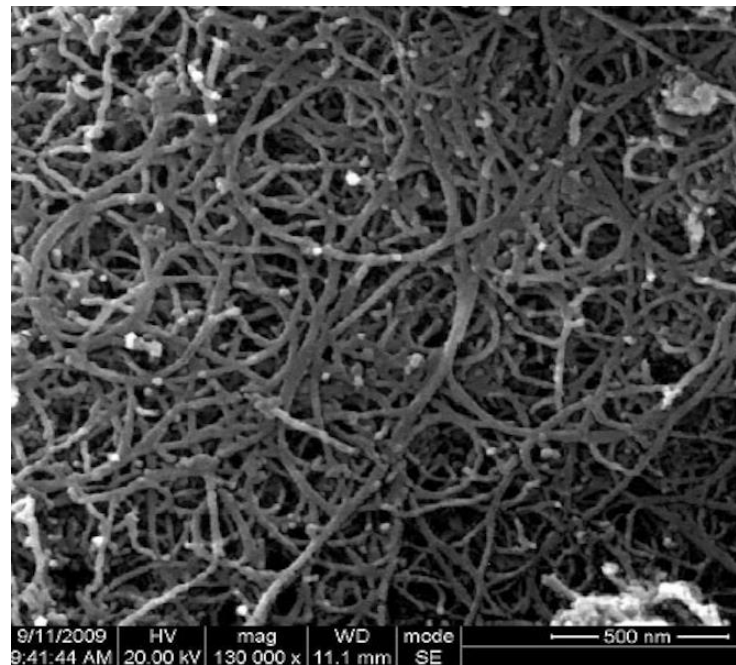
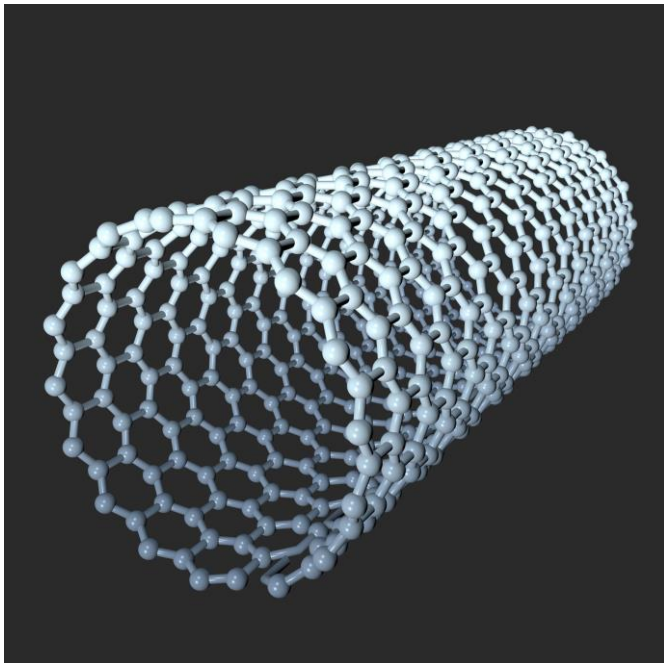
② 一维电子气 (第一个能带) : $k_F = \pi n/2$, $E_F = \hbar^2 k_F^2/2m_e$,

$$D(E) = \frac{2m_e}{\hbar \pi \sqrt{2m_e E}}$$

3.2 量子阱、量子线与量子点

3. 量子线

③ 实际体系一：碳纳米管

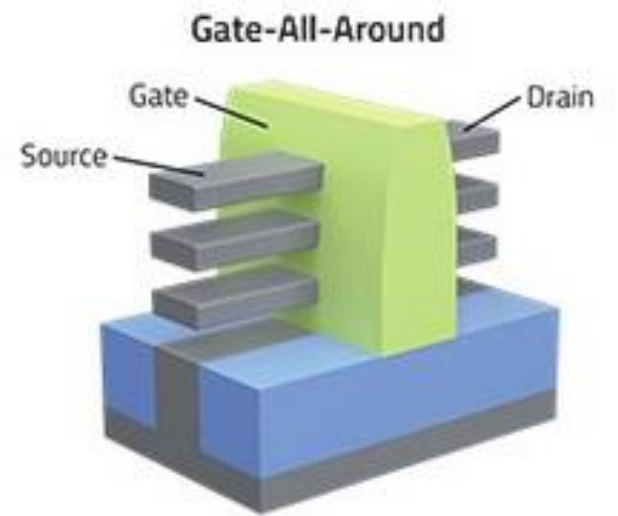
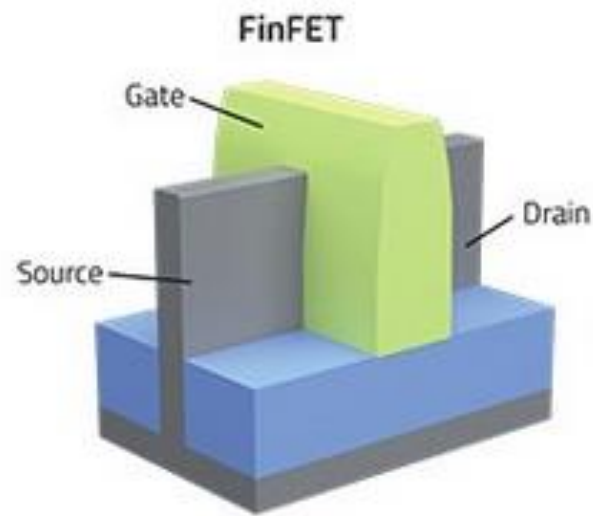
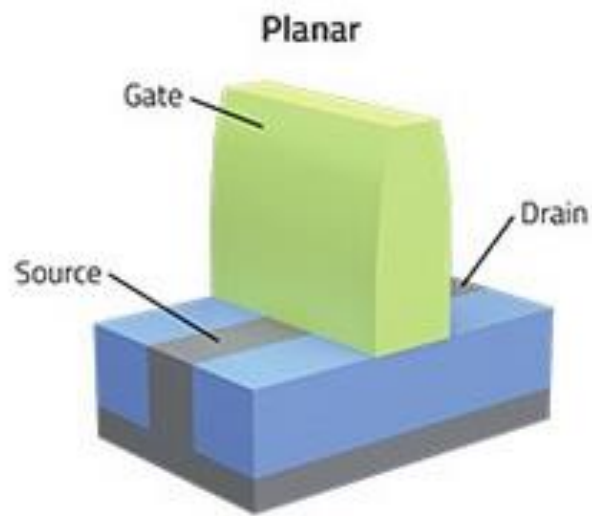


机械特性好、弹道输运

3.2 量子阱、量子线与量子点

3. 量子线

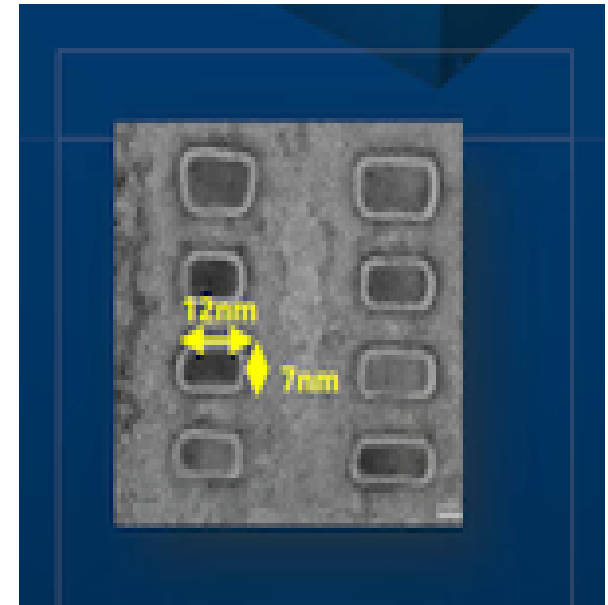
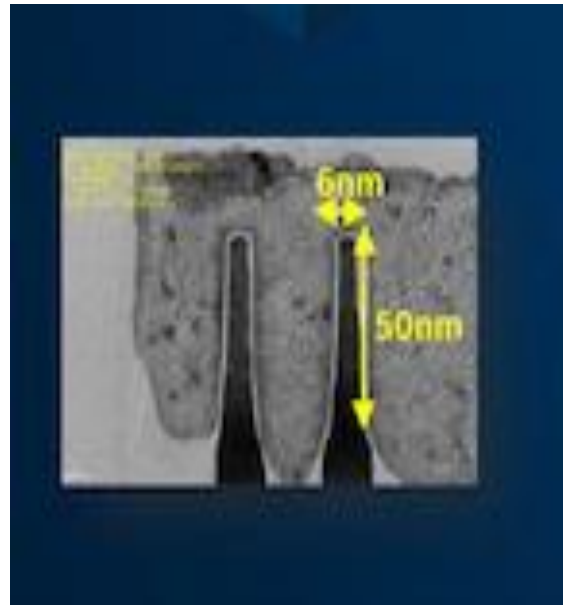
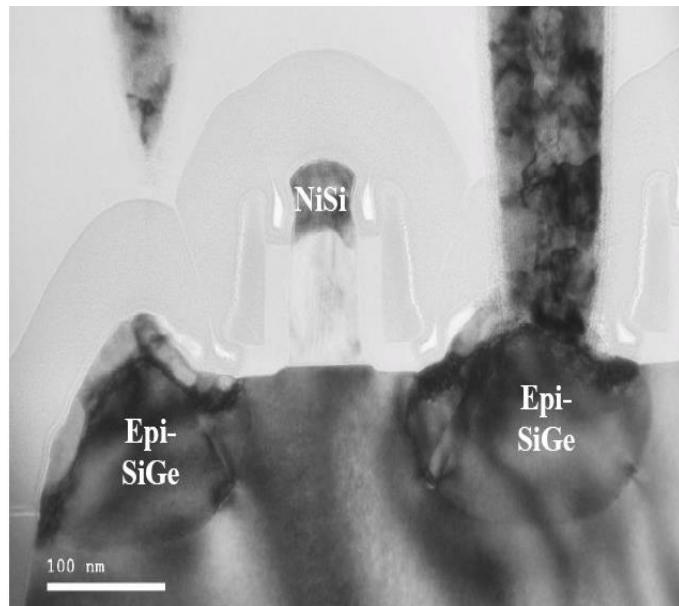
④ 实际体系二：GAA



3.2 量子阱、量子线与量子点

3. 量子线

④ 实际体系二：GAA



3.2 量子阱、量子线与量子点

3. 量子线

④ 实际体系二：GAA

| Gate-All-Around Transistor Deployment | | | |
|---------------------------------------|-----------|----------|-----------|
| AnandTech | Name | Process | Timeframe |
| Intel | RibbonFET | 20A | 2024 |
| | | 18A | 2025 |
| TSMC | GAAFET | N2 / 2nm | EoY 2023? |
| Samsung | MBCFET | 3GAE | 2022 |
| | | 3GAP | 2023 |

3.2 量子阱、量子线与量子点

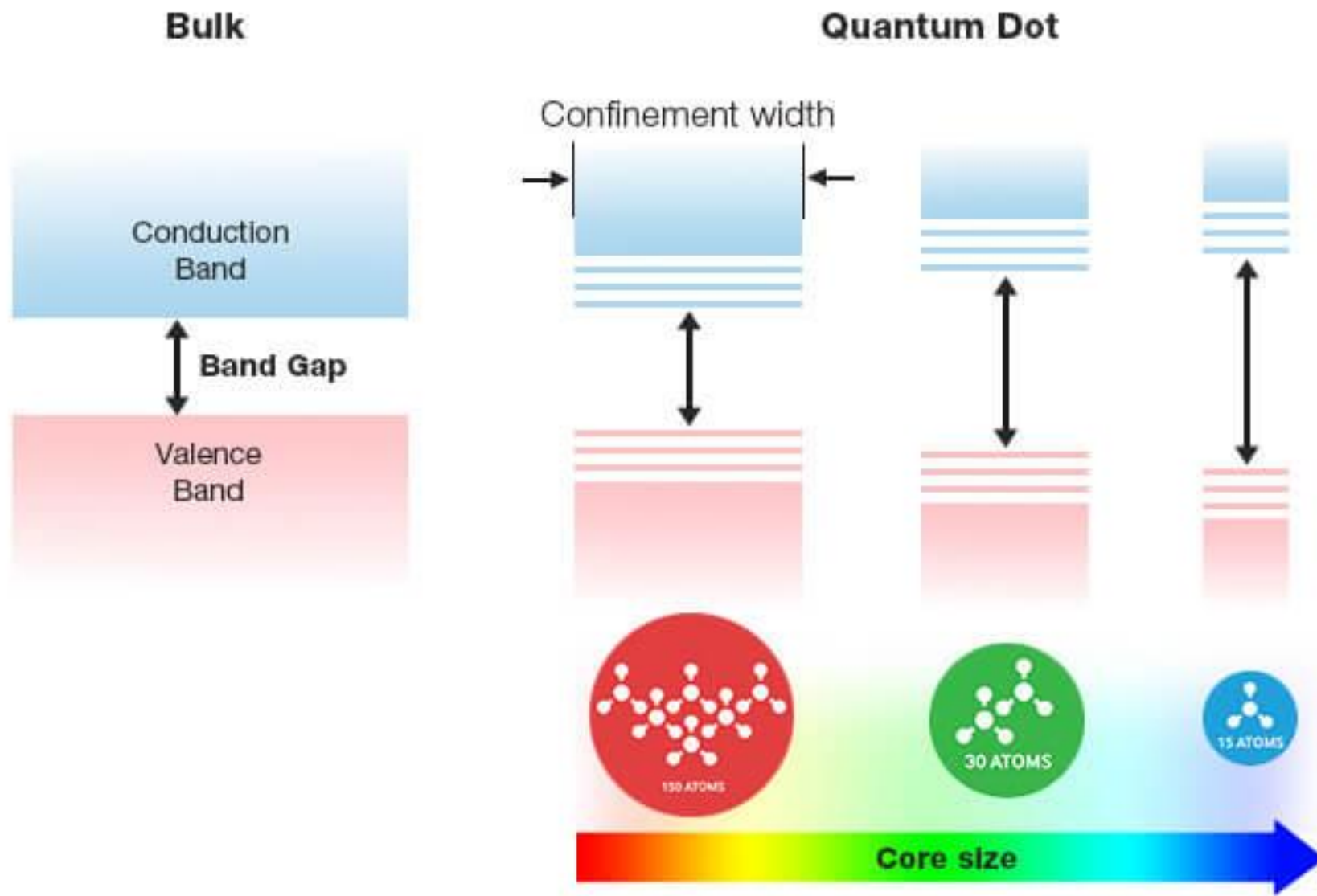
4. 量子点

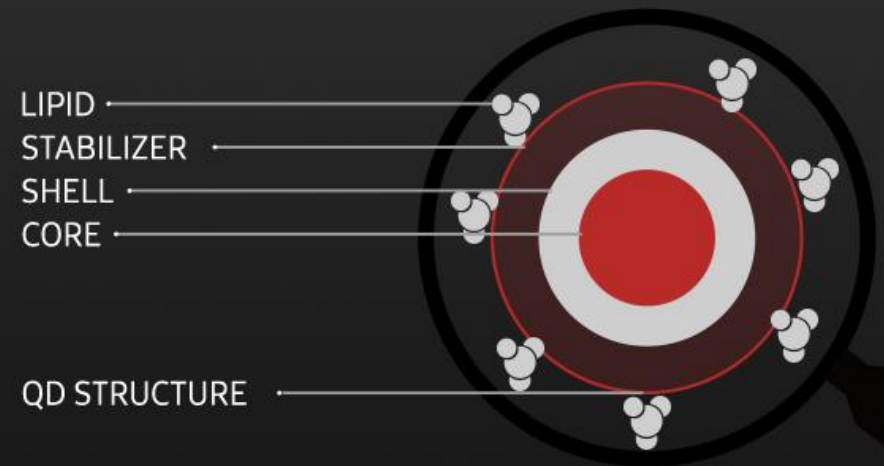
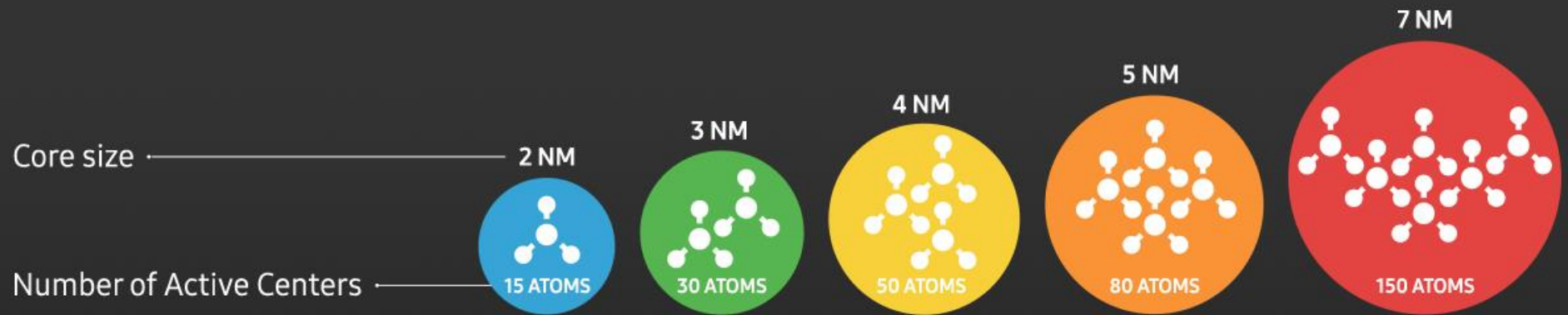
① xyz方向均受限

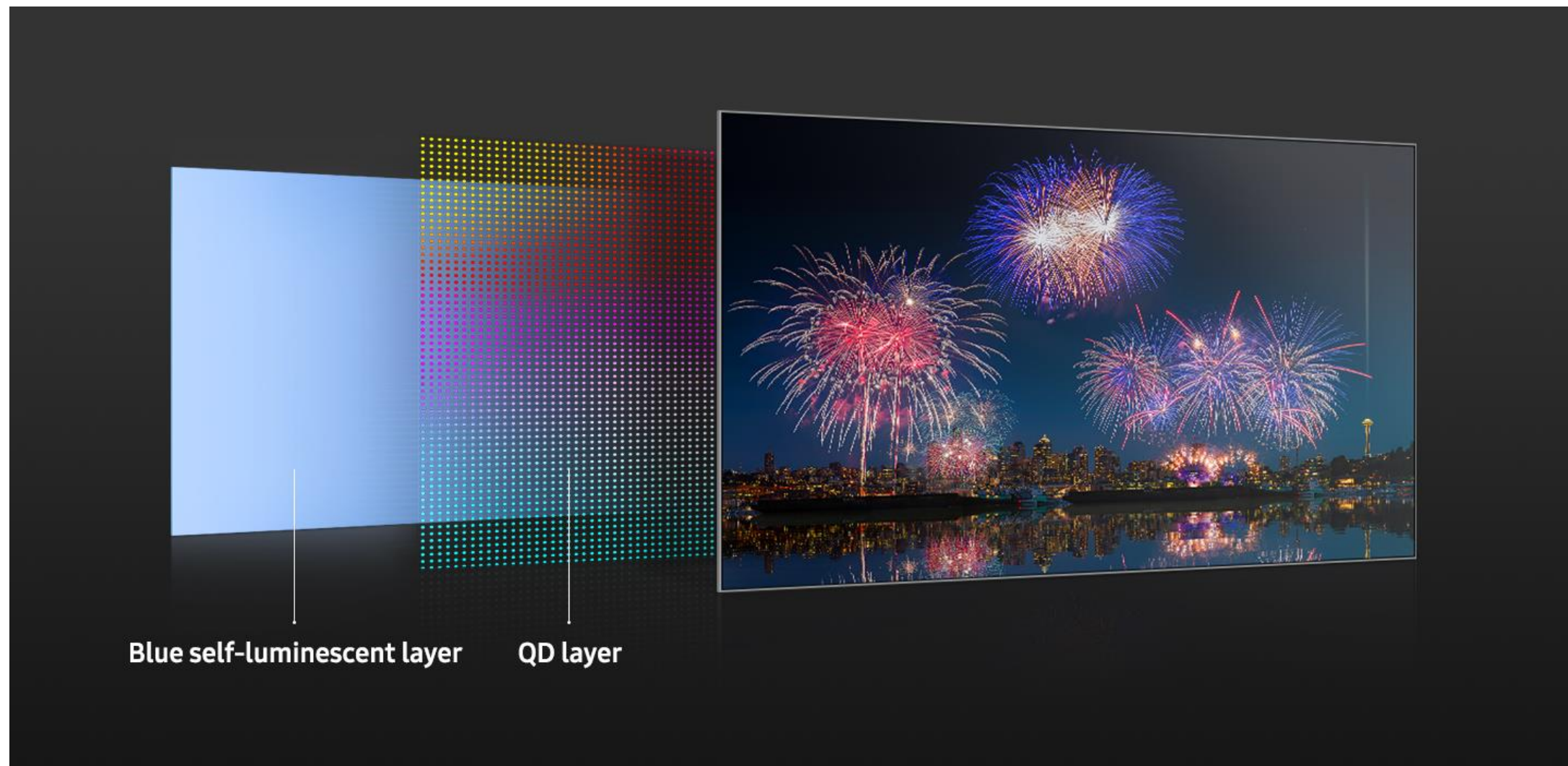
$$\psi_{m,n,l}(\mathbf{r}) = \sin\left(\frac{m\pi}{W_x}x\right) \sin\left(\frac{n\pi}{W_y}y\right) \sin\left(\frac{l\pi}{W_z}z\right),$$

$$E_{m,n,l} = \frac{\hbar^2 \left[\left(\frac{m\pi}{W_x}\right)^2 + \left(\frac{n\pi}{W_y}\right)^2 + \left(\frac{l\pi}{W_z}\right)^2 \right]}{2m_e}, \quad m,n,l \text{取值所有正整数}$$

② 量子点显示







<https://www.samsungdisplay.com/eng/tech/quantum-dot.jsp>