复习纲要

（基础理论部分）

李元

2025.04.10

Chapter 1

Crystal Structure
(晶体结构)

Chapter 1. Crystal Structure (晶体结构)

➢ **重要知识点**

Chapter 1.1: Periodic Array of Atoms (原子的周期性排列)

❖ Crystal Lattice (晶格)

❖ Lattice Vectors (格矢)

❖ Primitive Cell (原胞)

❖ Unit Cell (单胞)

❖ Miller Index (密勒指数)

Chapter 1. Crystal Structure (晶体结构)

➢ **重要知识点**

Chapter 1.2: Symmetry of Crystals (晶体的对称性)

❖ Macroscopic Symmetry of Crystals (晶体的宏观对称性)

❖ Symmetry Operations (对称操作)

❖ Symmetry Elements (对称元素)

❖ Point Groups (点群)

❖ Crystal Systems (晶系)

❖ Bravais Lattices (布拉维格子)

Chapter 1. Crystal Structure (晶体结构)

➢ **重要知识点**

Chapter 1.3: Typical Crystal Structures (典型晶体结构)

❖ Close Packing (密堆积)

       Hexagonal Close Packing (六角密堆, "HCP")

       Cubic Close Packing (立方密堆, or face-centered cubic, "FCC"):

❖ Simple Lattice and Compound Lattice (简单晶格与复式晶格)

❖ Important Crystal Structures (重要晶体结构)

       Simple Cubic, Body-Centered Cubic, Face-Centered Cubic, Diamond Structure

Chapter 1. Crystal Structure (晶体结构)

➢ **重要知识点**

Chapter 1.4: Reciprocal Lattice (倒易点阵)

❖ Reciprocal Lattice Vectors (倒格矢)

❖ Relationships between Reciprocal and Direct Lattices (倒格子与正格子的关系)

❖ Brillouin Zones (布里渊区)

Chapter 2

Crystal Binding
(晶体的结合)

Chapter 2. Crystal Binding (晶体的结合)

➢ **重要知识点**

❖ Fundamental Types of Crystal Binding (晶体结合的基本类型)

❖ Binding Energy (结合能)

❖ Ionic Binding (离子型结合)

❖ Covalent Binding (共价型结合)

❖ Metallic Binding (金属型结合)

Chapter 2. Crystal Binding (晶体的结合)

➤ **重要知识点**

Appendix 1: Basics of Quantum Mechanics (量子力学基础)

❖ Wave Function (波函数)

❖ Operators of Observables (力学量算符)

❖ Superposition Principle (态叠加原理)

❖ Schrodinger Equation (薛定谔方程)

❖ Identical Particles (全同粒子)

❖ Heisenberg Uncertainty Principle (海森堡不确定性原理)

Chapter 3

Lattice Vibrations and Phonons
(晶格振动与声子)

Chapter 3. Lattice Vibrations and Phonons (晶格振动与声子)

➤ **重要知识点**

Chapter 3.1: Classical Lattice Vibrations (晶格振动的经典理论)

❖ Vibrations of a 1D Monoatomic Chain (一维单原子链的振动)

❖ Vibrations of a 1D Diatomic Chain (一维双原子链的振动)

❖ Characteristics of Lattice Vibrations in 3D (三维晶格振动的特点)

➢ **重要知识点**

Chapter 3.2: Phonons (声子)

❖ Quantization of Lattice Vibrations (晶格振动的量子化)

❖ Phonons (声子)

➢ **重要知识点**

Chapter 3.3: Phonon Heat Capacity (声子热容)

❖ The Einstein Model (爱因斯坦模型)

❖ The Debye Model (德拜模型)

❖ Density of States (态密度)

➢ **重要知识点**

Appendix 3: Quantum Harmonic Oscillator (量子谐振子)

❖ Algebraic Method (代数解法)

Chapter 4

Electron Band Theory
(电子能带理论)

➤ **重要知识点**

Chapter 4.1: Nearly-Free-Electron Model (近自由电子模型)

❖ Bloch Theorem (布洛赫定理)

❖ Nearly-Free-Electron Model in 1D (一维近自由电子模型)

❖ The Difference between NFE Models in 1D and 3D (一维与三维近自由电子模型的区别)

➢ **重要知识点**

Chapter 4.2: Tight-Binding Model (紧束缚模型)

❖ Method of Linear Combination of Atomic Orbitals (原子轨道线性组合法)

❖ Tight-Binding Model in 1D (一维紧束缚模型)

❖ TB Model vs NFE Model (紧束缚模型与近自由电子模型的对比)

> **重要知识点**

Chapter 4.3: Square-Potential-Well Model (方势阱模型)

❖ Infinite Potential Well in 1D (一维无限深势阱)

❖ Finite Potential Barrier in 1D (一维有限高势垒)

Chapter 4. Electron Band Theory (电子能带理论)

➢ **重要知识点**

Chapter 4.4: Conductors & Nonconductors (导体与非导体)

❖ Characteristics of Electronic Wave Packets (电子波包的特点)

❖ Density of States and Fermi Surface (态密度与费米面)

❖ Fermi Energy and Fermi Level (费米能与费米能级)

❖ Classification of Conductors and Nonconductors (导体与非导体的分类)

➢ **重要知识点**

Appendix 4: Stationary Perturbation Theory (定态微扰论)

❖ Non-degenerate Perturbation Theory (非简并微扰论)

❖ Degenerate Perturbation Theory (简并微扰论)

Chapter 5

Metals and Semiconductors
(金属与半导体)

Chapter 5. Metals and Semiconductors (金属与半导体)

➤ **重要知识点**

Chapter 5.1: Free-Electron Theory of Metals (金属自由电子论)

❖ Classical Free-Electron Theory (经典自由电子论)

❖ Quantum Free-Electron Theory (量子自由电子论)

❖ Wiedemann-Franz Law (维德曼-夫兰兹定律)

❖ Work Function and Contact Potential (功函数与接触势)

Chapter 5. Metals and Semiconductors (金属与半导体)

> **重要知识点**

Chapter 5.2: Electron Theory of Semiconductors (半导体电子论)

❖ Band Gap (带隙)

❖ Charge Carriers (载流子)

❖ Dopants (掺杂物)

❖ Intrinsic and Extrinsic Semiconductors (本征与非本征半导体)

祝大家考试顺利！