$\boldsymbol{k} \cdot \boldsymbol{p}$ Perturbation and Energy Bands of Semiconductors

C. Hamaguchi

Professor Emeritus of Osaka University

Advanced Technology Research Laboratories, Sharp Corporation,

2613-1 Ichinomoto-cho, Tenri, Nara 632-8567, Japan

e-mail: hamaguchi-c@r6.dion.ne.jp

INTRODUCTION TO $\boldsymbol{k} \cdot \boldsymbol{p}$ PERTURBATION THEORY

Dresselhaus *et al.* [1] and Luttinger and Kohn [2], [3] introduced $\boldsymbol{k} \cdot \boldsymbol{p}$ perturbation theory to analyze the valence band structure of Ge and Si and later Kane [4], [5] extended $\boldsymbol{k} \cdot \boldsymbol{p}$ theory to include conduction bands. Cardona and Pollak [6] proposed $\boldsymbol{k} \cdot \boldsymbol{p}$ perturbation method to calculate energy bands in Ge and Si. In this lecture, the $\boldsymbol{k} \cdot \boldsymbol{p}$ perturbation theory is discussed in detail. First we show the energy band calculations of Ge and Si in the Brillouin zone and then we will show how to implement the spin–orbit interaction. In the second part we will discuss the analysis of the valence bands based on the second order perturbation of $\boldsymbol{k} \cdot \boldsymbol{p}$ Hamiltonian and the valence band parameters are determined. In the last part we discuss Luttinger Hamiltonian so called 4×4 (heavy and light hole bands), 6×6 (heavy, light and spin–orbit split off valence bands), and 8×8 (including the lowest conduction band) Luttinger Hamiltonian [7].

ENERGY BAND CALCULATIONS BY $\boldsymbol{k} \cdot \boldsymbol{p}$ THEORY

Schrödinger equation for an electron in a crystal is written as

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\boldsymbol{r}) \right] \Psi(\boldsymbol{r}) = \mathcal{E} \Psi(\boldsymbol{r}). \qquad (1)$$

The eigen function Ψ is given by Bloch function

$$\Psi(\boldsymbol{r}) = u_{\boldsymbol{k}}(\boldsymbol{r}) \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r}) \qquad (2)$$

where $u_{\boldsymbol{k}}(\boldsymbol{r})$ is a periodic function and $\boldsymbol{k}$ is the wave vector. Putting Eq. (2) into Eq. (1), we obtain

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\boldsymbol{r}) + \frac{\hbar}{m}(\boldsymbol{k} \cdot \boldsymbol{p}) \right] u_{n,\boldsymbol{k}}(\boldsymbol{r})$$
$$= \left(\mathcal{E}_n(\boldsymbol{k}) - \frac{\hbar^2 k^2}{2m} \right) u_{n,\boldsymbol{k}}(\boldsymbol{r}) \qquad (3)$$

Above equation reduces to $[H_0 + V(\boldsymbol{r})]u_{\boldsymbol{k}}(\boldsymbol{r}) = \mathcal{E}_n(0)u_{\boldsymbol{k}}(\boldsymbol{r})$ for $\boldsymbol{k} = 0$ which gives the eigen states at the Γ point. When we know the eigen states at $\boldsymbol{k} = 0$ we may obtain the eigen states $\boldsymbol{k} \neq 0$ by treating $H_1 = (\hbar/m)\boldsymbol{k} \cdot \boldsymbol{p}$ as a perturbing term.

The first part of this lecture deals with the following items.

1.1 Derivation of $\boldsymbol{k} \cdot \boldsymbol{p}$ Hamiltonian.

1.2 Determination of 15×15 matrix of $\boldsymbol{k} \cdot \boldsymbol{p}$ Hamiltonian and of the parameters.

1.3 Eigen states obtained by 15×15 pseudopotential Hamiltonian matrix.

1.4 Energy band calculations.

The second part will deal the analysis of the valence bands and derivation of Luttinger Hamiltonian.

2.1 Second order $\boldsymbol{k} \cdot \boldsymbol{p}$ perturbation.

2.2 Spin–orbit interaction.

2.3 6×6 $\boldsymbol{k} \cdot \boldsymbol{p}$ matrix of Dresselhaus *et al.*

2.4 6×6 $\boldsymbol{k} \cdot \boldsymbol{p}$ Luttinger Hamiltonian.

2.5 8×8 $\boldsymbol{k} \cdot \boldsymbol{p}$ Luttinger Hamiltonian.

CONCLUSION

This lecture gives an introduction to $\boldsymbol{k} \times \boldsymbol{p}$ perturbation theory to understand the energy band structures of semiconductors. The theory is used to analyze quantum structures such quantum well, quantum dot and quantum dot superlattices.

REFERENCES

[1] G. Dresselhaus: A.F. Kip, and C. Kittel: Phys. Rev. **98** (1955) 368

[2] J.M. Luttinger and W. Kohn: Phys. Rev. **97** (1955) 869

[3] J.M. Luttinger: Phys. Rev. **102** (1956) 1030

[4] E.O. Kane: J. Phys. Chem. Solids, **1** (1956) 82

[5] E.O. Kane: J. Phys. Chem. Solids **1** (1957) 249

[6] M. Cardona and F.H. Pollak: Phys. Rev. **142** (1966) 530

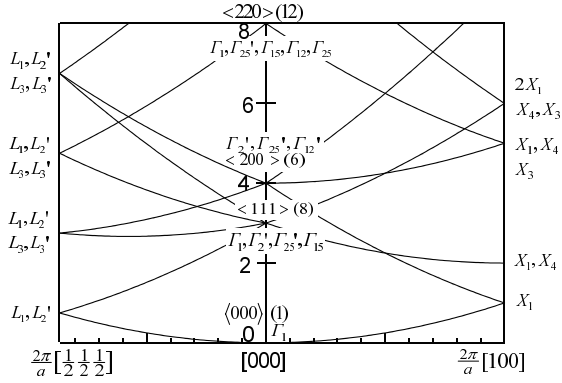[7] C. Hamaguchi: ”*Basic Semiconductor Physics*”, (Springer 2010), Chapter 1 and Chapter 2.

Fig. 1. Empty lattice bands of fcc crystals, where the degeneracy in the parentheses and the representations are shown.
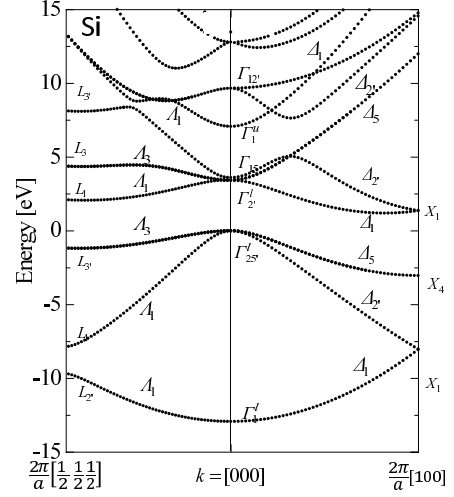

Fig. 4. Energy band structure of Si calculated by 15×15 $\boldsymbol{k} \cdot \boldsymbol{p}$ method.
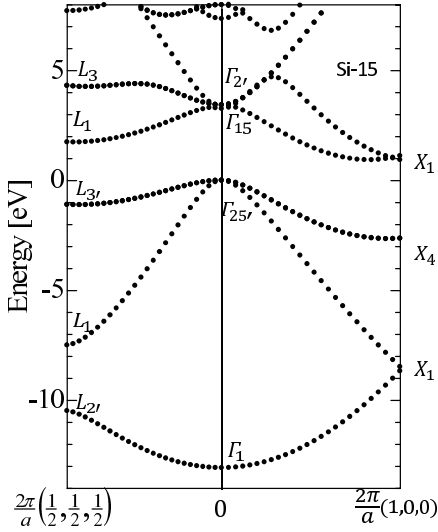

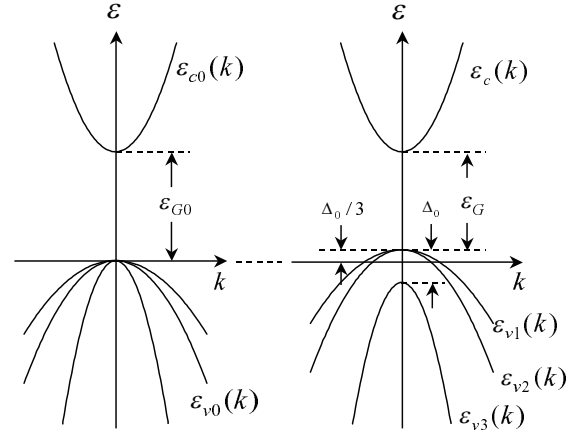Fig. 2. Energy band structure of Si calculated by empirical pseudopotential method with 15 plane waves.

Fig. 5. Valence band structure. The left figure is without spin–orbit interaction and the right figure shows the bands with spin–orbit interaction.
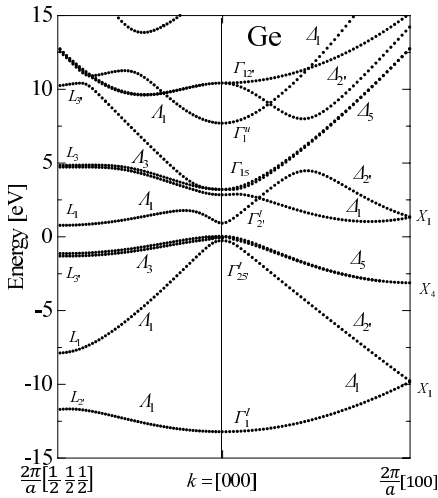

Fig. 3. Energy band structure of Ge calculated by 15×15 $\boldsymbol{k} \cdot \boldsymbol{p}$ method with spin–orbit interaction.
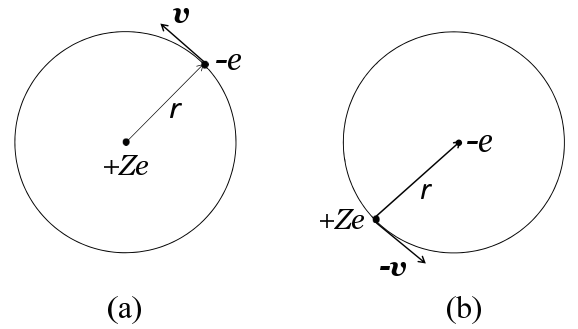

Fig. 6. (a) Bohr orbital motion of an electron $-e$ with the velocity $\boldsymbol{v}$ as seen by the nucleus Ze is interpreted from the point of view of the electron as (b) the nucleus Ze is moving with velocity $-\boldsymbol{v}$ around the electron.