Numerical Simulation of the Band structure of Silicon

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Introduction

Modern electronics relies on silicon, whose semiconducting properties are explained by its band structure. This structure describes how an electron's energy varies with its crystal momentum $\hbar\underline{k}$. The size and nature of the band gap determine whether silicon behaves as a metal, semiconductor, or insulator.

In this project we numerically solve the Schrödinger equation in a plane-wave basis to compute the band structure of silicon and compare it with experimental data.

To obtain the band structure we solve the Schrödinger equation for electrons in the periodic potential of the silicon lattice. In a periodic potential, Bloch's theorem states that electron states can be written as plane waves labelled by a wavevector k. Since the crystal potential $V(\mathbf{r})$ is periodic, this allows us to express the wavefunction as

$$\psi_k(\mathbf{r}) = \sum_{\mathbf{G}} a_{\mathbf{G}}(\mathbf{k}) \exp(i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r})$$

Here, $\mathbf{G}$ represents the reciprocal lattice vectors of the crystal. Substituting this into the Schrödinger equation and integrating over the unit cell transforms it into a matrix eigenvalue problem.

$$\begin{array}{c} \\ \mathbf{G} \\ \downarrow \end{array} \begin{array}{c} \mathbf{G} \quad \rightarrow \\ \left[\frac{\hbar^2|\mathbf{k}+\mathbf{G}|^2}{2m_e}\delta_{\mathbf{G}-\mathbf{G}'} + V_{\mathbf{G}-\mathbf{G}'} \right] \end{array} \begin{pmatrix} a_{\mathbf{G}\,1} \\ \vdots \\ a_{\mathbf{G}\,N} \end{pmatrix} = E_k \begin{pmatrix} a_{\mathbf{G}\,1} \\ \vdots \\ a_{\mathbf{G}\,N} \end{pmatrix} \tag{1}$$

$\mathbf{G}$ and $\mathbf{G}'$ here represent the reciprocal lattice vectors of silicon. Silicon has a face-centred cubic (FCC) Bravais lattice. Its reciprocal lattice vectors can be written as

$$\mathbf{G} = \frac{2\pi}{a}(h,k,l)$$

where (h,k,l) are integers with the same parity, either all even or all odd. The potential $V_{\mathbf{G}}$ is then defined:

$$V_{\mathbf{G}-\mathbf{G}'} = S\left(\mathbf{G}-\mathbf{G}'\right)\cdot V\left(\left|\mathbf{G}-\mathbf{G}'\right|\right) \tag{2}$$

$$S(\mathbf{G}) = \cos\left[\frac{\pi}{4}(h+k+l)\right]$$

where $V(|\mathbf{G}|)$, the form factor, is an empirically defined function, describing the Fourier components of the potential, as a function of $|\mathbf{G}|^2$.

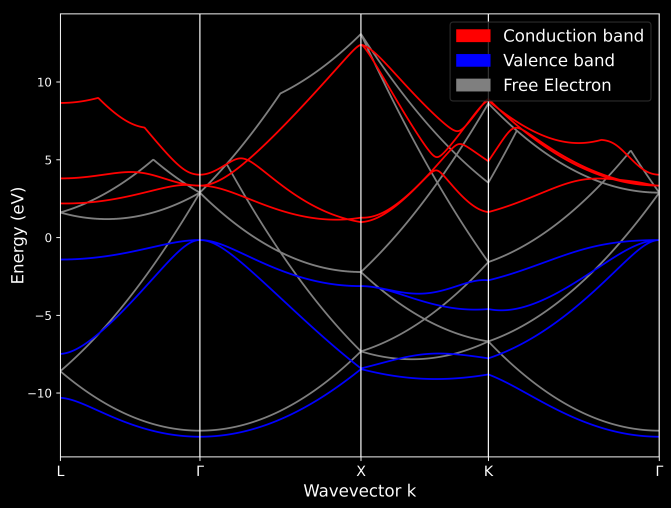

Figure 1: Calculated band structure. The path $L-\Gamma$-X-K-Γ connects standard high-symmetry points in k space.

Methods

Equation (1) was numerically implemented using a plane-wave basis truncated to 51 reciprocal lattice vectors, corresponding to $|\mathbf{G}|^2 \leq 11$. This cut-off offered a good balance between computational cost and accuracy. The lattice constant was set to $a = 5.43$ Å. The Fourier coefficients (in eV) from [3] used were:

$$V_3 = -3.04768,\ V_8 = 0.74831,\ V_{11} = 0.97961.$$

Matrix elements without a corresponding V value were set to zero, resulting in a sparse matrix. Matrices were constructed for each $\mathbf{k}$-point along the high-symmetry path Γ–X–W–L–Γ–K within the first Brillouin zone of the face-centred-cubic lattice.

Initially, to verify the algorithm's correctness, a free electron simulation was performed where all $V_i = 0$. This yielded Γ-point energies of 0 eV, 15.3 eV, and 20.4 eV, which correspond correctly to $\mathbf{G}$s of $(0,0,0)$, $(\pm1,\pm1,\pm1)$, and $(\pm2,0,0)$.

Eigenvalues were obtained by diagonalising the resulting Hermitian matrix using numpy's linalg.eigvalsh, and this procedure was repeated over 800 k-points to achieve a smooth energy dispersion curve.

Similarly, energy levels were sampled in the Brillouin zone unit cell at a resolution of $64 \times 64 \times 64$ to create Figure 2.

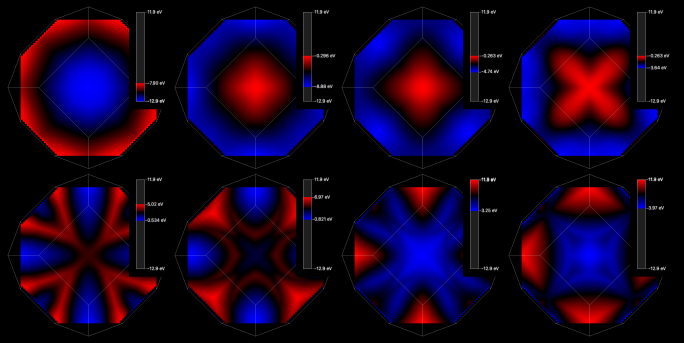

Figure 2: Cross-sections of the first eight energy bands across the Brillouin zone, showing the variation of energy with k.

Results

Eigenvalues were computed at 800 $\mathbf{k}$-points along the high-symmetry paths of the Brillouin zone. From this, an indirect band gap of 1.15 eV was obtained, which falls within the experimental range of 1.11–1.17 eV for temperatures between 0 and 300 K [2]. The valence band maximum is located at Γ, while the conduction band minimum lies on the Γ–X line. The resulting band structure is shown in Figure 1 and exhibits good qualitative agreement with the plot from [1]. Figure 2 presents a cross section of the first eight energy levels throughout the Brillouin zone.

Further Work

Our current method enables a more detailed characterisation of silicon. Specifically, we can also determine effective masses for electrons through parabolic fits near the band extrema, and compare these results with experimental data. Similarly, we can extend our study to germanium or gallium arsenide too.

References

[1] S. Yoshida et al., "Fundamental Properties of Wide Bandgap Semiconductors," in Wide Bandgap Semiconductors, K. Takahashi, A. Yoshikawa, and A. Sandhu, eds., Springer, Berlin, Heidelberg, 2007, p. 30, doi: 10.1007/978-3-540-47235-3_2.

[2] S. T. Thornton and A. Rex, Modern Physics for Scientists and Engineers, 4th ed., Boston, MA: Cengage Learning, 2020, ISBN 978-1-337-91945-6, ch. 11.2, p. 403.

[3] J. R. Chelikowsky and M. L. Cohen, "Electronic structure of silicon," Phys. Rev. B, vol. 10, p. 5095, Dec. 15, 1974, doi: 10.1103/PhysRevB.10.5095.

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