

Theory of Direct Optical Transitions in an Optical Indirect Semiconductor with a Superlattice Structure

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Abstract. Starting from a model of an indirect optical semiconductor with two bands, the electron states are calculated in the presence of an additional periodic one-dimensional potential (superlattice) in the semiconductor material. These states are used to determine the transition probability connected with the absorption of a photon. This transition corresponds to an optical direct transition – no phonon takes part in this process. The optical direct and optical indirect transitions are compared. For optical frequencies near the band gap one expects only direct transitions, whereby the optical indirect transitions may be neglected.

Index Headings: Superlattice – Optical transitions

In 1970 an IBM-group [1, 2] treated the electrical transport properties in a one-dimensional superlattice. In the meantime optical properties of a superlattice material in the microwave region have been examined theoretically [3–5], and some groups [6–9] started to construct such superlattice crystals.

A one-dimensional superlattice potential in a host crystal would be obtained by a periodic variation of the alloy composition or of the impurity density introduced during the epitaxial growth. The period of the superlattice must be shorter than the electron mean free path. Then one expects minizones in the momentum space, not observed in the host crystal [1, 2].

The present paper deals with the optical properties of an optical indirect host crystal (e.g. $\text{Si}_{1-x}\text{Ge}_x$) with a one-dimensional superlattice potential obtained by variation of the alloy composition.

For a period of the superlattice which is twice the lattice constant we give an exact treatment of the band structure of the superlattice crystal in terms of the host crystal. For simplicity we restrict ourselves

to a two-band model for the host crystal. Using the exact states of the former superlattice crystal, the transition probability connected with the absorption of a photon and the excitation of an electron from the upper valence band to the lower conduction band is calculated in first-order perturbation theory. This transition corresponds to optical direct transitions – no phonon is absorbed or emitted. The transition probabilities of the optical direct and indirect (second-order perturbation theory) transitions are compared. For optical frequencies near the band gap (near the infrared region for a $\text{Si}_{1-x}\text{Ge}_x$ -superlattice crystal) we expect only direct transitions, whereby the optical indirect transition may be neglected.

1. Hamiltonian for the Electrons in the Superlattice Crystal

We consider a two-band model of an alloy (compounds A and B) with a primitive cubic lattice. The minimum of the conduction band is assumed in the [100]-direction at the edge of the first Brillouin zone (Fig. 2). The Hamiltonian $H_0(r)$ for the electrons in

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the host crystal of the superlattice potential reads

$$H_0(\mathbf{r}) \varphi_{n,\mathbf{k}}(\mathbf{r}) = \varepsilon_n(\mathbf{k}) \varphi_{n,\mathbf{k}}(\mathbf{r}), \quad (1)$$

$$\varepsilon_n(\mathbf{k}) = \varepsilon_n(\mathbf{k} + \mathbf{K}), \quad (2)$$

$$\varphi_{n,\mathbf{k}}(\mathbf{r}) = \varphi_{n,\mathbf{k} + \mathbf{K}}(\mathbf{r}), \quad (3)$$

where n , \mathbf{k} and \mathbf{K} are the band index, wave vector in the first Brillouin zone, and a reciprocal lattice vector of the host crystal, respectively. The function $\varphi_{n,\mathbf{k}}(\mathbf{r})$ is the wave function, and $\varepsilon_n(\mathbf{k})$ is the corresponding energy eigenvalue of the host crystal.

By periodic variation of the alloy composition during the epitaxial growth in the $[100]$ -direction we obtain a one-dimensional superlattice crystal. The Hamiltonian for the electrons in this superlattice crystal contains now an additional term, the periodic superlattice potential $V_S(\mathbf{r})$.

$$(H_0(\mathbf{r}) + V_S(\mathbf{r})) \tilde{\varphi}(\mathbf{r}) = E \tilde{\varphi}(\mathbf{r}). \quad (4)$$

For simplicity, we restrict ourselves to a period of the superlattice which is twice the lattice constant a of the host crystal, i.e.

$$V_S \left(\mathbf{r} + \begin{pmatrix} 2a \\ 0 \\ 0 \end{pmatrix} \right) = V_S(\mathbf{r}). \quad (5)$$

The energy eigenvalue problem (4) of the electrons in the superlattice crystal may be represented by the Bloch functions of the unperturbed crystal, i.e.

$$\tilde{\varphi}(\mathbf{r}) = \sum_{n,\mathbf{k}} c_n(\mathbf{k}) \varphi_{n,\mathbf{k}}(\mathbf{r}), \quad (6)$$

$$\sum_{n',\mathbf{k}'} \{ (\varepsilon_{n'}(\mathbf{k}') - E) \delta_{n,n'} \delta_{\mathbf{k},\mathbf{k}'} + V_{nn'}(\mathbf{k},\mathbf{k}') \} c_{n'}(\mathbf{k}') = 0, \quad (7)$$

$$V_{nn'}(\mathbf{k},\mathbf{k}') = \int_V d^3\mathbf{r} \varphi_{n,\mathbf{k}}^*(\mathbf{r}) V_S(\mathbf{r}) \varphi_{n',\mathbf{k}'}(\mathbf{r}). \quad (8)$$

Using Bloch's theorem

$$\varphi_{n,\mathbf{k}}(\mathbf{r}) = \frac{1}{N} e^{i\mathbf{k}\mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r}), \quad (9)$$

$$\int_V d^3\mathbf{r} u_{n,\mathbf{k}}^*(\mathbf{r}) u_{n',\mathbf{k}'}(\mathbf{r}) = \delta_{n,n'} \quad (10)$$

(N , Δv and $u_{n,\mathbf{k}}(\mathbf{r})$ are defined in the host crystal consisting of N unit cells with the volume Δv ; $u_{n,\mathbf{k}}(\mathbf{r})$ has the periodicity of the lattice of the host crystal in the ordinary space) the non vanishing

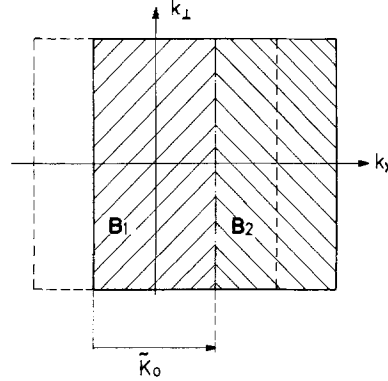


Fig. 1. Basic region in the k -space for the host crystal ($\mathbf{B}_1 \oplus \mathbf{B}_2$) and for the superlattice crystal (\mathbf{B}_1)

matrix elements $V_{nn'}(\mathbf{k},\mathbf{k}')$ read

$$V_{nn'}(\tilde{\mathbf{k}},\tilde{\mathbf{k}}) = \frac{1}{2} \int_V d^3\mathbf{r} u_{n,\tilde{\mathbf{k}}}^*(\mathbf{r}) V_S(\mathbf{r}) u_{n',\tilde{\mathbf{k}}}(\mathbf{r}), \quad (11)$$

$$V_{nn'}(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0, \tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0) = \frac{1}{2} \int_V d^3\mathbf{r} u_{n,\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0}^*(\mathbf{r}) V_S(\mathbf{r}) u_{n',\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0}(\mathbf{r}), \quad (12)$$

$$V_{nn'}(\tilde{\mathbf{k}}, \tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0) = \frac{1}{2} \int_V d^3\mathbf{r} u_{n,\tilde{\mathbf{k}}}^*(\mathbf{r}) V_S(\mathbf{r}) u_{n',\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0}(\mathbf{r}), \quad (13)$$

$$V_{nn'}(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0, \tilde{\mathbf{k}}) = V_{n'n}^*(\tilde{\mathbf{k}}, \tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0). \quad (14)$$

Here

$$\tilde{\mathbf{K}}_0 = \frac{\pi}{a} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad (15)$$

is the shortest reciprocal lattice vector in the $[100]$ -direction of the superlattice crystal, and ΔV is the volume of a unit cell of the superlattice crystal consisting of two unit cells of the host crystal.

In deriving (11) to (14) we used a range of the wave vectors \mathbf{k} and \mathbf{k}' in (7) and (8) (equivalent to the first Brillouin zone), which was obtained by shifting the first Brillouin zone by the vector $1/2 \cdot \tilde{\mathbf{K}}_0$. This new range for the wave vectors may be divided into two subranges \mathbf{B}_1 and \mathbf{B}_2 (see Fig. 1).

The wave vector $\tilde{\mathbf{k}}$ defined in the region \mathbf{B}_1 (corresponding to the first Brillouin zone of the superlattice crystal) is given by the wave vector \mathbf{k} defined in the regions \mathbf{B}_1 and \mathbf{B}_2

$$\left. \begin{aligned} \mathbf{k} &= \tilde{\mathbf{k}} & \text{for } \mathbf{k} \in \mathbf{B}_1 \\ \mathbf{k} &= \tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0 & \text{for } \mathbf{k} \in \mathbf{B}_2. \end{aligned} \right\} \quad (16)$$

The matrix elements (11) to (14) are restricted by the conservation of the wave vectors up to the shortest reciprocal lattice vector $\tilde{\mathbf{K}}_0$ of the superlattice crystal.

2. Bandstructure of the Superlattice Crystal in the [100]-Direction

For wave vectors in the [100]-direction we assume the Bloch functions which in the valence- and the conduction bands are representations of the “little” group \mathbf{G}_k (containing all symmetry operations of the host crystal transforming the [100]-direction into itself). If the superlattice potential $V_S(\mathbf{r})$ commutes with all symmetry elements of the “little” group \mathbf{G}_k and the representation of the valence- and conduction bands belongs to *different* irreducible representations of the little group \mathbf{G}_k , then all matrix elements $V_{nn'}(\mathbf{k}, \mathbf{k}')$ vanish with $n \neq n'$.

The diagonal matrix elements $V_{nn}(\tilde{\mathbf{k}}, \tilde{\mathbf{k}})$ and $V_{nn}(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0, \tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0)$ may be included in the energy eigenvalues of the host crystal $\varepsilon_n(\tilde{\mathbf{k}})$ and $\varepsilon_n(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0)$, respectively.

The eigenvalue problem (7) of the superlattice crystal reads now

$$\left. \begin{aligned} [\varepsilon_n(\tilde{\mathbf{k}}) - E] c_n(\tilde{\mathbf{k}}) + M_{nn}^*(\tilde{\mathbf{k}}) c_n(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0) &= 0, \\ [\varepsilon_n(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0) - E] c_n(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0) &= 0, \end{aligned} \right\} \quad (17)$$

$$\left. \begin{aligned} + M_{nn}(\tilde{\mathbf{k}}) c_n(\tilde{\mathbf{k}}) &= 0, \\ V_{nn}(\tilde{\mathbf{k}}, \tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0) &= M_{nn}(\tilde{\mathbf{k}}), \\ V_{nn}(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0, \tilde{\mathbf{k}}) &= M_{nn}^*(\tilde{\mathbf{k}}). \end{aligned} \right\} \quad (18)$$

This energy eigenvalue problem is solved by

$$E_n^\pm(\tilde{\mathbf{k}}) = \frac{1}{2} \{ \varepsilon_n(\tilde{\mathbf{k}}) + \varepsilon_n(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0) \pm [\Delta \varepsilon_n^2(\tilde{\mathbf{k}}) + 4|M_{nn}(\tilde{\mathbf{k}})|^2]^{1/2} \}, \quad (19)$$

$$\Delta \varepsilon_n(\tilde{\mathbf{k}}) = \varepsilon_n(\tilde{\mathbf{k}}) - \varepsilon_n(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0), \quad (20)$$

$$\tilde{\varphi}_{n,\tilde{\mathbf{k}}}^\pm(\mathbf{r}) = c_n^\pm(\tilde{\mathbf{k}}) \varphi_{n,\tilde{\mathbf{k}}}(\mathbf{r}) + c_n^\pm(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0) \varphi_{n,\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0}(\mathbf{r}), \quad (21)$$

$$c_n^\pm(\tilde{\mathbf{k}}) = \frac{e^{i\varphi_n^\pm}}{\sqrt{2}} \left(1 \pm \frac{\Delta \varepsilon_n(\tilde{\mathbf{k}})}{[\Delta \varepsilon_n^2(\tilde{\mathbf{k}}) + 4|M_{nn}(\tilde{\mathbf{k}})|^2]^{1/2}} \right)^{\pm 1/2}, \quad (22)$$

$$c_n^\pm(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0) = \mp \frac{e^{i\varphi_n^\pm}}{\sqrt{2}} \left(1 \mp \frac{\Delta \varepsilon_n(\tilde{\mathbf{k}})}{[\Delta \varepsilon_n^2(\tilde{\mathbf{k}}) + 4|M_{nn}(\tilde{\mathbf{k}})|^2]^{1/2}} \right)^{\pm 1/2} \quad (23)$$

$$\left. \begin{aligned} e^{i\varphi_n^+} &= 1, \\ e^{i\varphi_n^-} &= \frac{M_{nn}(\tilde{\mathbf{k}})}{|M_{nn}(\tilde{\mathbf{k}})|}. \end{aligned} \right\} \quad (24)$$

Here $E_n^\pm(\tilde{\mathbf{k}})$ (see Fig. 2) is the energy eigenvalue and $\tilde{\varphi}_{n,\tilde{\mathbf{k}}}^\pm(\mathbf{r})$ the corresponding eigenfunction of the Hamiltonian (4) for the electrons in the superlattice crystal. In the model considered one band of the host crystal

induces two bands (“mini-bands”) of the superlattice crystal.

If we fix the phases of the coefficients $c_n^\pm(\tilde{\mathbf{k}})$ and $c_n^\pm(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0)$ according to (24), we obtain for $V_S(\mathbf{r}) \rightarrow 0$ ($M_{nn} \rightarrow 0$, $\Delta \varepsilon > 0$):

$$\left. \begin{aligned} c_n^+(\tilde{\mathbf{k}}) &\rightarrow 1; & c_n^-(\tilde{\mathbf{k}}) &\rightarrow 0 \\ c_n^+(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0) &\rightarrow 0; & c_n^-(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0) &\rightarrow 1 \end{aligned} \right\} \quad (25)$$

or

$$\left. \begin{aligned} \tilde{\varphi}_{n,\tilde{\mathbf{k}}}^+(\mathbf{r}) &\rightarrow \varphi_{n,\tilde{\mathbf{k}}}(\mathbf{r}), \\ \tilde{\varphi}_{n,\tilde{\mathbf{k}}}^-(\mathbf{r}) &\rightarrow \varphi_{n,\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0}(\mathbf{r}). \end{aligned} \right\} \quad (26)$$

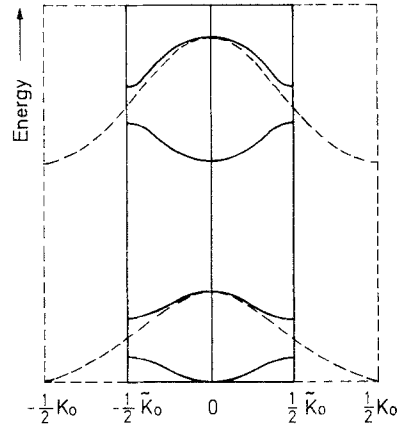


Fig. 2. Bandstructure of the superlattice crystal (solid line) and the band structure of the host crystal (dashed line) in the [100]-direction

3. Optical Transitions in the Superlattice Crystal

We are now interested in optical transitions near the band gap of the superlattice crystal. Therefore we may restrict ourselves to small wave vectors $\tilde{\mathbf{k}}$. Assuming $u_{n,\tilde{\mathbf{k}}}(\mathbf{r})$ defined in (9) as a slowly varying function of $\tilde{\mathbf{k}}$, we approximate $u_{n,\tilde{\mathbf{k}}}(\mathbf{r})$ and $u_{n,\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0}(\mathbf{r})$ by $u_{n,0}(\mathbf{r})$ and $u_{n,\tilde{\mathbf{K}}_0}(\mathbf{r})$.

The Hamiltonian of the electron-photon interaction is given by

$$H_{eF}(\mathbf{r}) = -\frac{e}{mc} \mathbf{A}(\mathbf{r}) \cdot \mathbf{p}, \quad (27)$$

where $\mathbf{A}(\mathbf{r})$ is the vector potential of the electromagnetic field ($\text{div } \mathbf{A} = 0$) and \mathbf{p} is the operator of the electron momentum. Assuming the electromagnetic field to be a plane wave with the frequency ω_λ , the wave vector \mathbf{k}_λ and the polarization \mathbf{e}_λ , $\mathbf{A}(\mathbf{r})$ may be written as

$$\mathbf{A}(\mathbf{r}) = \sqrt{\frac{2\pi c^2 \hbar}{\omega_\lambda V}} \mathbf{e}_\lambda (b_\lambda^+ e^{-i\mathbf{k}_\lambda \cdot \mathbf{r}} + b_\lambda e^{i\mathbf{k}_\lambda \cdot \mathbf{r}}), \quad (28)$$

where b_λ^+ and b_λ denote the creation – and annihilation operator for photons in the mode λ .

The transition probability $W_{c^-,v^+}(\tilde{\mathbf{k}}, \tilde{\mathbf{k}}')$ per unit time for a electron transition in the superlattice crystal from the upper valence band v^+ to the lowest conduction band c^- by absorption of a photon is given by

$$W_{c^-,v^+}(\tilde{\mathbf{k}}, \tilde{\mathbf{k}}') = \frac{4\pi^2 e^2 N_\lambda}{m^2 \omega_\lambda V} \delta(E_v^+(\tilde{\mathbf{k}}') + \hbar\omega_\lambda - E_c^-(\tilde{\mathbf{k}})) \cdot \left| \int_V d^3 r \tilde{\varphi}_{c,\tilde{\mathbf{k}}}^-(\mathbf{r}) e^{i\mathbf{k}_\lambda \cdot \mathbf{r}} \mathbf{e}_\lambda \cdot \mathbf{p} \tilde{\varphi}_{v,\tilde{\mathbf{k}}'}^+(\mathbf{r}) \right|^2, \quad (29)$$

where N_λ is the number of photons in the mode λ . Using (21) the matrix element in (29) responsible for the optical transitions reads

$$\int d^3 r \tilde{\varphi}_{c,\tilde{\mathbf{k}}}^-(\mathbf{r}) e^{i\mathbf{k}_\lambda \cdot \mathbf{r}} \mathbf{e}_\lambda \cdot \mathbf{p} \tilde{\varphi}_{v,\tilde{\mathbf{k}}'}^+(\mathbf{r}) = \delta_{\tilde{\mathbf{k}}, \tilde{\mathbf{k}}' + \mathbf{k}_\lambda} \tilde{O}_{c^-,v^+}(\tilde{\mathbf{k}}), \quad (30)$$

$$\begin{aligned} \tilde{O}_{c^-,v^+}(\tilde{\mathbf{k}}) &= c_c^{*-}(\tilde{\mathbf{k}}) c_v^+(\tilde{\mathbf{k}} - \mathbf{k}_\lambda) (O_{cv}(\tilde{\mathbf{k}}) \\ &\quad + \mathbf{e}_\lambda \cdot (\tilde{\mathbf{k}} - \mathbf{k}_\lambda) O'_{cv}(\tilde{\mathbf{k}})) \\ &\quad + c_c^{*-}(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0) c_v^+(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0 - \mathbf{k}_\lambda) \\ &\quad \cdot (O_{cv}(\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0) \\ &\quad + \mathbf{e}_\lambda \cdot (\tilde{\mathbf{k}} + \tilde{\mathbf{K}}_0 - \mathbf{k}_\lambda) O'_{cv}(\tilde{\mathbf{k}} + \tilde{\mathbf{K}})), \end{aligned} \quad (31)$$

$$O_{cv}(\mathbf{k}) = \int_{\Delta v} d^3 r u_{c,\mathbf{k}}^*(\mathbf{r}) \mathbf{e}_\lambda \cdot \mathbf{p} u_{v,\mathbf{k}-\mathbf{k}_\lambda}(\mathbf{r}), \quad (32)$$

$$O'_{cv}(\mathbf{k}) = \int_{\Delta v} d^3 r u_{c,\mathbf{k}}^*(\mathbf{r}) \cdot u_{v,\mathbf{k}-\mathbf{k}_\lambda}(\mathbf{r}). \quad (33)$$

The quantity $\tilde{O}_{c^-,v^+}(\tilde{\mathbf{k}})$ is the matrix element for optical transitions in the superlattice crystal, whereas $O_{cv}(\mathbf{k})$ and $O'_{cv}(\mathbf{k})$ describe the matrix elements for optical transitions in the host crystal.

For simplicity we assume $O_{cv}(\mathbf{k}) \neq 0$, the small matrix elements $O'_{cv}(\mathbf{k})$ may then be neglected.

The total transition probability $W_{c^-,v^+}^{(d)}$ per unit time for absorption of a photon in the superlattice crystal is given by summing up (29) over all initial and final states, i.e.

$$W_{c^-,v^+}^{(d)} = \sum_{\tilde{\mathbf{k}}, \tilde{\mathbf{k}}'} 2 W_{c^-,v^+}(\tilde{\mathbf{k}}, \tilde{\mathbf{k}}') [1 - n_{c^-}(\tilde{\mathbf{k}})] n_{v^+}(\tilde{\mathbf{k}}'). \quad (34)$$

Here $n_{v^+}(\tilde{\mathbf{k}})$ is the probability for an occupied initial electron state in the valence band, whereas $[1 - n_{c^-}(\tilde{\mathbf{k}})]$ describes the probability of an empty final electron state in the conduction band. The factor 2 takes into account the two spin directions of every electron state $\{n^\pm, \tilde{\mathbf{k}}\}$.

For room temperature and a band gap of about 1 eV we have

$$\begin{aligned} n_{c^-}(\tilde{\mathbf{k}}) &= 0 \\ n_{v^+}(\tilde{\mathbf{k}}) &= 1. \end{aligned} \quad (35)$$

Using (29) and (35) the total transition probability per unit time (34) for absorption of a photon reads

$$W_{c^-,v^+}^{(d)} = \int d^3 \mathbf{k} \frac{e^2 N_\lambda}{\pi m^2 \omega_\lambda} \cdot \delta(E_v^+(\tilde{\mathbf{k}} - \mathbf{k}_\lambda) + \hbar\omega_\lambda - E_c^-(\tilde{\mathbf{k}})) |\tilde{O}_{c^-,v^+}(\tilde{\mathbf{k}})|^2. \quad (36)$$

Optical transitions near the band edge restrict us to small wave vectors $\tilde{\mathbf{k}}$. As discussed above, $u_{n,\tilde{\mathbf{k}}}(\mathbf{r})$ and $u_{n,\tilde{\mathbf{k}}+\tilde{\mathbf{K}}_0}(\mathbf{r})$ are slowly varying functions of $\tilde{\mathbf{k}}$. Therefore the optical matrix elements (31), $\tilde{O}_{c^-,v^+}(\tilde{\mathbf{k}})$, may be approximated by $\tilde{O}_{c^-,v^+}(0)$.

Neglecting in $E_v^+(\tilde{\mathbf{k}} - \mathbf{k}_\lambda)$ of (36) the small wave vector \mathbf{k}_λ of the absorbed photon and assuming for $E_v^+(\tilde{\mathbf{k}})$ and $E_c^-(\tilde{\mathbf{k}})$ the effective mass approximation the integral in (36) may be stated as

$$E_c^-(\tilde{\mathbf{k}}) = \varepsilon_G + \frac{\hbar^2 \tilde{\mathbf{k}}^2}{2m_{c^-}} \quad (37)$$

$$E_v^+(\tilde{\mathbf{k}}) = -\frac{\hbar^2 \tilde{\mathbf{k}}^2}{2m_{v^+}},$$

$$\begin{aligned} W_{c^-,v^+}^{(d)} &= |\tilde{O}_{c^-,v^+}(0)|^2 \frac{2e^2 N_\lambda}{m^2} \left(\frac{\bar{m}}{\hbar^2} \right)^{\frac{3}{2}} \\ &\quad \cdot \frac{(\hbar\omega_\lambda - \varepsilon_G)^{\frac{1}{2}}}{\omega_\lambda} \Theta(\hbar\omega - \varepsilon_G), \end{aligned} \quad (38)$$

$$\Theta(x) = \begin{cases} 1 & \text{for } x > 0 \\ 0 & \text{for } x < 0. \end{cases} \quad (39)$$

The quantity \bar{m} in (38) is defined as

$$\frac{2}{\bar{m}} = \frac{1}{m_{v^+}} + \frac{1}{m_{c^-}}. \quad (40)$$

For a band structure with anisotropic effective masses near the band edge only the factor $\bar{m}^{\frac{3}{2}}$ is changed in (38).

The optical matrix element (31), $\tilde{O}_{c^-,v^+}(0)$, of the superlattice crystal reads in terms of the optical matrix elements (32), $O_{cv}(0)$ and $O_{cv}(\tilde{\mathbf{K}}_0)$, of the host crystal

$$\tilde{O}_{c^-,v^+}(0) = \frac{M_{cc}^*(0)}{\Delta \varepsilon_c(0)} O_{cv}(0) - \frac{M_{vv}^*(0)}{\Delta \varepsilon_v(0)} O_{cv}(\tilde{\mathbf{K}}_0). \quad (41)$$

In deriving (41) the roots of the coefficients $c_n^\pm(0)$ and $c_n^\pm(\tilde{\mathbf{K}}_0)$ defined in (21) and (22) are approximated by

($|M| \approx 0.1$ eV, $\Delta\varepsilon \approx 1$ eV):

$$\left. \begin{aligned} \left(1 + \frac{1}{(1+x^2)^{\frac{1}{2}}}\right)^{\frac{1}{2}} &= \sqrt{2} + O(x^2) \\ \left(1 - \frac{1}{(1+x^2)^{\frac{1}{2}}}\right)^{\frac{1}{2}} &= \frac{1}{\sqrt{2}}x + O(x^3) \end{aligned} \right\} \quad (42)$$

$$x^2 = 4 \frac{|M_{nn}(0)|^2}{\Delta\varepsilon_n^2(0)} \ll 1. \quad (43)$$

4. Comparison of the Optical Direct and Indirect Transitions

Following the paper of Bardeen, Blatt and Hall [10] the total transition probability $W_{c,v}^{(i)}$ per unit time for absorption of a photon in an optical indirect semiconductor reads

$$\begin{aligned} W_{c,v}^{(i)} &= \left| \frac{O_{cv}(\vec{K}_0) P_{vv}}{\Delta\varepsilon_v(0)} - \frac{O_{cv}(0) P_{cc}}{\Delta\varepsilon_c(0)} \right|^2 \frac{e^2 N_\lambda}{\pi m^2} V N_c \\ &\cdot n_P \frac{(\hbar\omega_\lambda + \hbar\Omega - \varepsilon_G)^2}{\omega_\lambda} \\ &+ \Theta(\hbar\omega_\lambda - \hbar\Omega - \varepsilon_G) (n_P + 1) \frac{(\hbar\omega_\lambda - \hbar\Omega - \varepsilon_G)^2}{\omega_\lambda} \Big\}, \end{aligned} \quad (44)$$

$$Q = A \frac{2(\hbar\omega_\lambda/\varepsilon_G - 1)^{\frac{1}{2}} \Theta(\hbar\omega - \varepsilon_G)}{(\hbar\omega_\lambda/\varepsilon_G - 1 + \hbar\Omega/\varepsilon_G)^2 + (\hbar\omega_\lambda/\varepsilon_G - 1 - \hbar\Omega/\varepsilon_G)^2 \Theta(\hbar\omega_\lambda - \varepsilon_G - \hbar\Omega)}, \quad (47)$$

$$A = \frac{2}{N_c} \frac{m^{*2} \bar{m}^{\frac{1}{2}} l |M_{cc}(0)|^2}{(m_v^* m_c^*)^{\frac{1}{2}} \varepsilon_G^{\frac{3}{2}} \hbar}. \quad (48)$$

where P_{vv} and P_{cc} are matrix elements describing the electron-phonon interaction in the host crystal, $n_P(\Omega)$ is the number (frequency) of the phonons taking part in the process of an indirect optical transition, and N_c is the number of minima of the conduction band in the host crystal. In our model these minima are located at the edge of the first Brillouin zone. Therefore we have only $N_c = 3$. If the corresponding minima are located inside the first Brillouin zone (e.g. of Si), we have $N_c = 6$.

We want to give a rough estimate of the ratio Q defined by

$$Q = \frac{W_{c,v}^{(d)}}{W_{c,v}^{(i)}}, \quad (45)$$

where $W_{c,v}^{(d)}$ and $W_{c,v}^{(i)}$ are determined by (38) and (44), respectively.

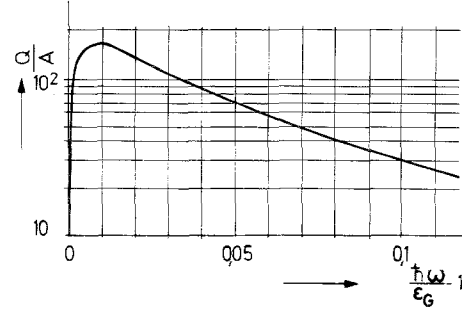


Fig. 3. The ratio Q of the transition probabilities of optical direct and indirect transitions as a function of the photon frequency ω ($\varepsilon_G \approx 1$ eV band gap; $\hbar\Omega \approx 1/40$ eV phonon energy)

For simplicity we neglect in $W_{c,v}^{(d)}$ and $W_{c,v}^{(i)}$ terms with the optical matrix elements $O_{cv}(\vec{K})$. Then the matrix element $O_{cv}(0)$ cancels, and the ratio Q is therefore independent of the optical matrix elements.

A rough estimate of the matrix element P_{cc} for the electron-phonon interaction in $W_{c,v}^{(i)}$ may be obtained from the mean free path l of the electrons [10]

$$\frac{1}{l} = 2n_P |P_{cc}|^2 V \frac{1}{\pi \hbar^4} m^{*2}. \quad (46)$$

Now the ratio Q of the transition probabilities $W_{c,v}^{(d)}$ and $W_{c,v}^{(i)}$ reads

With (e.g. for Si)

$$m^* = \bar{m} = m_v^* = m_c^* = 0.3 m_e \quad (m_e: \text{free electron mass})$$

$$l = 5 \cdot 10^{-6} \text{ cm}$$

$$|M_{cc}| = 0.1 \text{ eV}$$

$$\varepsilon_G = 1 \text{ eV}$$

$$N_c = 3$$

we obtain for A a value in the order of one, namely

$$A = 0.72. \quad (49)$$

At room temperature the energy $\hbar\Omega$ of the exited phonons assisting the optical indirect transition is of the order of $1/40$ eV. With this value of the phonon energy the function Q/A of the photon frequency ω_λ is given in Fig. 3.

As seen in Fig. 3, the direct optical transitions in the superlattice crystal dominate for optical frequencies

near the band gap. The corresponding transition probability is expected to be $10^1 - 10^2$ times the transition probability for the optical indirect transitions.

Experimental verifications (e.g. in a $\text{Si}_{1-x}\text{Ge}_x$ -superlattice crystal) of the results of these theoretical calculations will become important in new optical devices (laser diodes, luminescence diodes, etc.).

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Appendix

Some Aspects of a Generalization to Larger Periods of the Superlattice Potential

Assuming a superlattice potential of the form

$$V_s(r) = \frac{1}{2}(e^{iK_s r} + e^{-iK_s r}) \tilde{V}_s(r),$$

$$\tilde{V}_s(r + R) = \tilde{V}_s(r),$$

$$K_s = \begin{pmatrix} K_s^0 \\ 0 \\ 0 \end{pmatrix}; \quad K_s^0 = \frac{2\pi}{ma}; \quad m \approx 10 - 20,$$

where R means a lattice vector of the host crystal, and ma is the periodicity of the superlattice potential.

Following the calculation in Section 2 one can show that in the $[100]$ -direction a state $\{n, k\}$ of the host crystal is coupled due to the superlattice potential to the states $\{n, k \pm K_s\}$. The corresponding energy differences of the electrons in these states $[\varepsilon_n(k) - \varepsilon_n(k \pm K_s)]$ are expected to be smaller or of the same order of magnitude

as the matrix elements $V_{nn}(k, k \pm K_s)$ [see (8)] responsible for the coupling of these states. In this case the diagonalization of the Hamiltonian of the superlattice crystal (in the representation of the Bloch functions of the host crystal) by a perturbation technique fails.

In a perturbation-theoretical treatment the expansion parameter $V/\Delta\varepsilon$ is assumed to be small due to the convergence of this treatment. An analytically exact diagonalization of the mentioned Hamiltonian is not yet known. Nevertheless, one expects, due to the superlattice potential, an "indirect" coupling of the states $\{n, k \approx 0\}$ at the Γ -point and of the states $\{n; k \approx +K_0/2\}$ at the edge of the first Brillouin zone ($\{n, k\}$: states of the host crystal). Direct optical transitions in such crystals should be observed, too. The corresponding transition probability is expected to be high enough for optical devices.

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