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Infrared absorption, multiphonon processes and time reversal effect on Si and Ge band structure

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ABSTRACT

We have examined the effect of Time Reversal Symmetry (TRS) on vibrational modes and on the electronic band structure of Si and Ge. Most of the primary non-interacting modes are not affected by TRS. Only phonons originating from high symmetry lines S and A of the Brillouin Zone (BZ) indicate extra degeneracy. Selection rules for some two and three phonons originating from high symmetry lines are determined. The states of electrons and holes described by electronic band structure due to spin-inclusion are assigned by spinor representations of the double space group. Inclusion of the TRS into the band structure results in extra degeneracy of electrons and holes, and therefore optical selection rules suppose to be modified.

1. Introduction

Much attention has been devoted to infrared absorption (IR), Raman Scattering (RS) and multiphonon scattering processes in Diamond, Si and Ge over the last fifty years. The theory of IR and RS in Diamond structure has been developed by Birman [1]. Particularly, detailed analysis of IR and RS experimental data by means of group theoretical selection rules can be found in a comprehensive review book by Birman [2] where references to many experimental and theoretical data can be found. Also multiphonon processes in crystals with Diamond structure, as well as modern quantum theories of lattice Raman Scattering and infrared absorption have been studied (Chapters L and N) in [2]. However, not much attention has been directed to the effect of TRS on vibrational modes and electronic states determined by band structure in Si and Ge. It is the aim of this contribution to investigate the selection rules (SRs) for phonon processes originating from high symmetry lines in the Brillouin Zone (BZ) and electronic, optical transitions in the presence of TRS. In Sections 2.1, 2.2, 2.3, and 2.4 we recall the necessary theory of TRS regarded to the degeneracy of spinless particles and particles with spin 1/2, electrons and holes. In each subsection we apply theory to vibrational modes and electronic states in Si and Ge.

2. Space and Time Reversal Symmetry

2.1. Space symmetry. Spin excluded. Single value representations

Space symmetry of a crystal requires invariance of a Hamiltonian with respect to symmetry operator g belonging to a space group $G^{\mathbf{k}}$. Therefore, the eigenfunctions Ψ and $g\Psi$ correspond to the same energy. Consequently, the states are classified according to Single Valued Irreducible Representations D (SVIrrps) of a space group;

$$g \in G, g^{-1}Hg = H, \quad g\Psi_i = \sum_j D_{ji}(g)\Psi_j. \tag{1}$$

The dimension of the representation (dim D) indicates the degeneracy degree of states. Spin less quasi-particles such as phonons are well described by SVIrrp. The vibrational modes of Si and Ge are classified according to the following SVIrrps of $O_H^7(Fd3m)$ space group: $\Gamma_{25}{}'$ (Γ_{5+}), Γ_{15} (Γ_{4-}), Δ_1, Δ_2, Δ_5, Λ_1, Λ_2, Λ_3, Σ_1, Σ_2, Σ_3, W_1, W_2, L_1, L_2, L_3, X_1, X_2, X_3, X_4 those follow from the lattice Mode Representation and compatibilities along the high symmetry point and lines. The two and three phonon processes originating from the high symmetry points in Diamond structure (Si, Ge), have already been studied [2]. However, it is known that the phonon of high symmetry lines also contribute essentially to the phonon density of states (DOS) as do high symmetry point modes. Therefore, it is necessary to study the SRs for these phonons. Using standard group theoretical technique we have derived several selection rules for these phonons listed in Table 1. The labeling of irrps is in terms of Bouckaert et al. [3] and in brackets in terms of

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Table 1
Selection rules for phonons of high symmetry lines: Δ, Λ, Σ in Si and Ge[a]

Species	Type of resulting phonon symmetries
A. Two phonon processes. Overtones	
$[\Delta_1\ (A)]_2$	Γ_{4-} $(\Gamma_{15}$ (A)), Δ_1 (A), Σ_1 (A)
$[\Delta_2\ (O)]_2$	Γ_{5+} $(\Gamma_{25'}$ (O)), Δ_2 (O), Σ_1 (O)
$[\Delta_5\ (A)]_2$	Γ_{4-} $(\Gamma_{15}$ (A)), Δ_1 (A), Σ_1 (A), Σ_3 (A), Σ_4 (A)
$[\Delta_5\ (O)]_2$	Γ_{5+} $(\Gamma_{25'}$ (O)), Δ_2 (O), $2\Sigma_1$ (O), Σ_3 (O)
$[\Lambda_1\ (A)]_2$	Γ_{4-} $(\Gamma_{15}$ (A)), Δ_1(A), Σ_1(A)
$[\Lambda_1\ (O)]_2$	Γ_{5+} $(\Gamma_{25'}$ (O)), Σ_1(O))
$[\Lambda_3\ (A)]_2$	Γ_{5+} $(\Gamma_{25'}$ (A)), Δ_1(A) Δ_5 (A)
$[\Lambda_3\ (O)]_2$	Γ_{5+} $(\Gamma_{25'}$ (O)), Δ_2(O), Δ_5 (O)
$[\Sigma_{1,2,3}\ (A)]_2$	Γ_{4-} $(\Gamma_{15}$ (A)), Δ_1(A), Σ_1 (A)
$[\Sigma_{1,2,3}\ (O)]_2$	Γ_{5+} $(\Gamma_{25'}$ (O)), Δ_2 (O), Δ_5 (O), Σ_1(O)
B. Two phonon processes. Combination	
$\Delta_1 \otimes \Delta_2$	Δ_2 (O)
$\Delta_1 \otimes \Delta_5$	Δ_5 (A, O)
$\Delta_2 \otimes \Delta_5$	Δ_5 (A, O)
$\Delta_1 \otimes \Delta_3$	Δ_3 (A, O)
$\Sigma_1 \otimes \Sigma_2 = \Sigma_3 \otimes \Sigma_4$	Σ_2 (O)
$\Sigma_1 \otimes \Sigma_3 = \Sigma_2 \otimes \Sigma_4$	Σ_3 (A, O)
$\Sigma_1 \otimes \Sigma_4 = \Sigma_2 \otimes \Sigma_3$	Σ_4 (A, O)
C. Three phonon processes. Overtones	
$[\Delta_1\ (A)]_3$	Δ_2 (A), Δ_2 (O), Δ_1 (A), $2\Delta_3$ (A, O)
$[\Delta_2\ (O)]_3$	$2\Delta_2$ (O), Δ_1 (A), $2\Delta_3$ (A, O)
$[\Delta_5\ (A)]_3$	Δ_1 (A), Δ_2 (O), Δ_5 (A), Δ_5 (O)
$[\Delta_5\ (O)]_3$	Δ_1 (A), Δ_2 (O), Δ_5 (A), Δ_5 (O)
$[\Lambda_1]_3$	$2\Lambda_1$, $2\Lambda_3$
$[\Lambda_3]_3$	several modes of Λ_1, $2\Lambda_3$ symmetries
$[\Sigma_{1-4}]_3$	$\Gamma_{5+}(\Gamma_{25'}$(O)), $2\Gamma_{4+}(\Gamma_{15}$ (A)), Δ_1(A), Δ_5(A, O), $2\Delta_3$(A, O) Λ_1(A, O), $2\Lambda_3$ (A, O), $2\Sigma_1$(A, O)
D. Three phonon processes. Some combinations	
$\Delta_1 \otimes \Delta_1 \otimes \Gamma_{25'}(O) =$	$\Delta_1 \otimes \Delta_5 \Rightarrow \Delta_5$(A, O)
$\Delta_2 \otimes \Delta_2 \otimes \Gamma_{15}(A) =$	$\Delta_2 \otimes (\Delta_2 \oplus \Delta_5) = [\Delta_2]_2 \oplus \Delta_5$ (A, O)
$\Delta_5 \otimes \Delta_5 \otimes \Gamma_{25'}(O) =$	$\Delta_2 \otimes (\Delta_2 \oplus \Delta_5) = 2\Delta_5$ (A, O), $[\Delta_5]_2$, $\Delta_5 \otimes \Delta_5$
$\Delta_1 \otimes \Delta_1 \otimes \Gamma_{25'}(O) =$	......
$D^i \otimes D^j \otimes D^k =$	......
	i,j,k, $\Delta_{1,2,5}$, $\Lambda_{1,3}$, $\Sigma_{1,2,3,4}$, Γ_{15}, $\Gamma_{25'}$[b]

[a] In brackets are irrps labeled according to BSW [3], whereas $\Gamma_{4-,5+}$ are in CDML [4] notation.

[b] There are many three phonon combinations to be worked out. Our Table 1, regarding to high symmetry lines, is just an extension of Tables II and III for multiphonon processes in Si and Ge of Birman's work [2]. The selection rules in our Table 1, are governed by wavevector selection rules and KP of irrps species. For example, the KP $\Lambda_1 \otimes \Lambda_3 = \Lambda_3$ (A, O) means

$$\hbar g_i \boldsymbol{k}_\Lambda + \hbar g_j \boldsymbol{k}_\Lambda = \hbar \boldsymbol{k}_\Lambda \tag{6}$$

where $\hbar g_i \mathbf{k}_\Lambda$ and $\hbar g_i \mathbf{k}_\Lambda$ are arms of $\boldsymbol{k}_\Lambda$ k in the star $\{^*\boldsymbol{k}_\Lambda\}$ and $\boldsymbol{k}_\Lambda$ are the first wavevector of the star according to which the irrps of $G^k{}_\Lambda$ are tabulated [4]. Eq. (5) represents the momentum conservation principle, which corresponds to the KPs of Λ's irrps. From the interaction of Λ_1 and Λ_3 phonons described by KP; $\Lambda_1 \otimes \Lambda_3$, the resulting phonon is Λ_3(A, O), A acoustic or/and O optical.

Cracknell Davis Miller Love (CDML) [4]. For Ge phonons see Fig. 2 Lax and Hopfield [5].

SVIrrps are also used in the classification of electron and holes in band structure, provided negligible spin–orbit interaction. Nevertheless, frequently in many semiconductors spin–orbit interaction is quite appreciable. Moreover, when high crystalline specimen are illuminated, the creation of excitons takes place. Therefore, spin of electron and hole must be taken into account.

2.2. Space symmetry. Spin included. Double valued representations

Inclusion of electron spin in a crystal lattice results in double space group and its Double Valued Irreducible Representation (DVIrrps) [6]. In this case the states of electrons in the conduction band (CB) and holes in the valence band (VB) are classified according to the DVIrrps (Spinors). For the band structure in terms of DVIrrps of Ge and Si see Figures 2.13, 6.13 in [7,8]. The DVIrrps of Si and Ge in terms of CDML labeling are: $\Gamma_{6\pm,\ 7\pm,\ 8\pm}$, X_5, $L_{4\pm,\ 5\pm,\ 6\pm}$, $W_{3,4,5,6}$, $\Delta_{6,7}$, $\Lambda_{4,5,6}$, Σ_5, S_5, and $Z=V_{2,3,4,5}$. In Ge the minimum in the conduction band occurs at point L (L_1^+ SVIrrp [5] and L_{6+}, DVIrrp [4,8]), whereas the maximum in VB occurs at Γ ($\Gamma_{25'}$ SVIrrp) [3], Γ_{8+} (DVirrp) [4]. The appropriate selection rules for direct radiative transitions are: $\Gamma_{8+}(\mathrm{VB}) \otimes \Gamma_{7-}\ (\mathrm{CB}) \otimes \Gamma_{4-}$ (light symmetry)$= (\Gamma_{3-} \oplus \Gamma_{4-} \oplus \Gamma_{5-}) \otimes \Gamma_{4-}$. Because $\Gamma_{4-} \otimes \Gamma_{4-}$ contains Γ_1 (identity rep) the transition is allowed. However, the transition does not connect the desired states. The indirect phonon assisted transition $L_{6+} \otimes \Gamma_{8+} \otimes \Gamma_{4-} = (L_{1+} \oplus L_{2+} 3L_{3+}) \otimes \Gamma_{4-}$ is allowed, because the Kronecker Product contains the symmetry allowed phonons L_{1+}, L_{2+}, L_{3+}, those follow from compatibility relations $\Gamma \rightarrow L$ and wavevector selection rules (momentum conservation principle) $\hbar\vec{k}_\Gamma + \hbar\vec{k}_L = \hbar k_L$.

2.3. Time Reversal Symmetry for spinless particles

So far we have discussed rather well known space group theoretical SRs in the absence of TRS. However, many physical systems contain an invariance under the inversion of the direction of wave propagation or magnetic moment of a crystal. This is also true on quantum mechanical systems. In here we discuss the effect of TR operator for spinless quasi-particles, like phonons in Ge and Si. We consider only non-interacting modes discussed in the Section 2.1. For vibrational modes the energy operator H is real (no spin, no spin–orbit interaction, no magnetic field). The time dependent Schrödinger equation is invariant under time inversion. Taking the complex conjugation of time dependent Schrödinger equation we obtain:

$$H\psi = i\hbar\frac{\partial\psi}{\partial t}, t \rightarrow -t, (\ldots)^*, H\Psi^* = -i\hbar\frac{\partial\psi^*}{\partial(-t)} = i\hbar\frac{\partial\psi^*}{\partial t} = H\Psi^*. \tag{2}$$

Associating replacement t by $-t$ to a TR operator K, we have $K\Psi = \Psi^*$, the operator K transforms Ψ into Ψ^*. From Eq. (1) follows that Ψ^* is also an eigenfunction of H. The Ψ and Ψ^* belong to the same energy (eigenvalue). Since (Ψ,Ψ^*) transform according to complex conjugate reps D and D^* of the anti-unitary group G^{-k} it follows that

$$K(g\psi_i) = K\left(\sum_j D_{ji}\psi_j\right) = \sum D^*_{ji}(K\psi_i) = \sum D^*_{ji}\psi^*_i \Rightarrow, Kg = gK. \tag{3}$$

The wave functions (Ψ, Ψ^*) are the basis of D and D^* reps, respectively. If Ψ and Ψ^* are linearly dependent, $K\Psi_i = \Psi_i^* = \Sigma_j T_{ji}$, Ψ_j via unitary matrix T, then D and D^* are equivalent, $D \approx D^*$, $\chi(g) = \chi^*(g)$. In this case (a) TRS does not introduce an extra degeneracy. If Ψ and Ψ^* are linearly independent then they transform according to inequivalent reps D and D^* ($D \not\approx D^*$, $\chi(g) \neq \chi^*(g)$). In this case (b) the states (Ψ,Ψ^*) transform according to the joint reps $D \oplus D^*$.Clearly, an extra TRS degeneracy occurs. The linearly independent states can still transform according to equivalent reps D and D^*. In this case (c) the states $\phi$and ϕ^* also transform according to the joint rep $D \oplus D^*$, $D \approx D^*$, $\chi(g) = \chi^*(g)$. Again the TRS occurs. It is just a matter to find out whether or not the inclusion of TRS leads to an extra degeneracy. Fröbenius–Schur derived reality test for irrps [9]. Adjusted for space groups it is of the form

$$R = \frac{f}{h'}\sum_{g \in G^k} \chi_k(g^2)\delta_{k,-gk} = +1(\mathrm{a}), \quad -1(\mathrm{c}), \quad 0(\mathrm{b}) \tag{4}$$

$$g\vec{k} = -\vec{k} \tag{5}$$

where all the quantities have their usual meaning [10,11]. And summation is performed over the fundamental elements $g^2 \in G^k$ such that $g\mathbf{k} = -\mathbf{k}$. The eigenfunctions of vibrational modes are just harmonic displacement of atoms from their in equilibrium positions. They contain the time dependent factor and wave vector k which due

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to complex conjugation becomes $-k$. In other words, the direction of mode propagation changes from $+\boldsymbol{k}$ into $-\mathbf{k}$. And the star $\{{}^*\boldsymbol{k}\}$ of a space group changes into $-\{{}^*\boldsymbol{k}\}$. Using Eqs. (4), (5) we have tested all SVIrrpps of Si and Ge discussed in Section 2.1. We have found all irrps at high symmetry points Γ, L, X, W and lines Σ, Λ, Δ and Q real. Only S and A phonons are TRS degenerate. Generally, most of the pronounced vibrational modes in Si and Ge do not experience extra degeneracy by TRS inclusion. However, the TRS inclusion into the states of electrons and holes assignment in terms of band structure $E(\boldsymbol{k})$ leads to an essential degeneracy.

2.4. Time Reversal Symmetry for particles with 1/2 spin

As discussed in Section 2.2 the states of electrons and holes due to spin are classified according to the DVirrps. It can be shown that the TR operator for quantum mechanical system with spin 1/2 ($S_y = \frac{1}{2}\hbar\sigma_y$) for electrons, holes, etc. is of the form $T=-i\sigma_y K$, K is a complex conjugation operator. For electron Bloch wave functions with spin up and down, we have: $H\psi_{\vec{k}\uparrow}=E(\vec{k}\uparrow)\psi_{\vec{k}\uparrow}$, $\psi_{k\uparrow}=u_k(r)\exp(i\vec{k}\cdot\vec{r})\times$(spin-up function). In the presence of TRS, the Hamiltonian transforms as $T^{-1}HT=H$ for H real. If we operate by T on $\psi_{\vec{k}}\uparrow$ the Pauli spin operator will operate only on the spin function and will turn the spin-up function into a spin-down function; $\psi_{\vec{k}\uparrow}=i\sigma_y K\psi_{\vec{k}\uparrow}=i\exp(-i\vec{k}\cdot\vec{r})$ $u^*_{\vec{k}}(\vec{r})\times$(spin-down function). It follows that functions $\psi_{\vec{k}\uparrow}$ (up) and $\psi_{\vec{k}\downarrow}$ (down) must be degenerate owing to TRS. Consequently, an important result of TRS on electronic band structure is $E(\vec{k}\uparrow)=E(-\vec{k}\downarrow)$. If, in addition, the crystal has an inversion symmetry, then $E(\vec{k}\uparrow)=E(-\vec{k}\uparrow)$ because the space inversion operator takes k into $-k$ but does not operate on the spin. If TR and space inversion symmetries are simultaneously present in a crystal we have $E(\vec{k})=E(-\vec{k})$ for any spin. In the next section we discuss the consequences of TRS on states of particles with 1/2 spin.

2.5. Classification of particles states with spin in the presence of Time Reversal Symmetry

The basis function of DVirrps are Bloch functions with spin, $\psi_{\vec{k}}(\vec{r})\times$(spin function), where $\psi_{\vec{k}}(\vec{r})=\exp(i\vec{k}\cdot\vec{r})u_{\vec{k}}(\vec{r})$. In the presence of TRS there are two set of Bloch functions; $\psi_{\vec{k}\uparrow}$ and $T\psi_{\vec{k}\uparrow}=i\psi^*_{\vec{k}}\times$ (spin-down function). In other words, the electron states owing to TRS are classified now by joint reps $D^k\oplus(D^k)^*$. As in Section 2.3 these two wavefunctions can be linearly dependent. Then $(i\sigma_y K)\psi^j_{\vec{k}}=\Sigma_j T_{ji}\,\psi^j_{\vec{k}}$. In this case (a) there is no extra degeneracy and $D^{\vec{k}}\approx(D^{\vec{k}})^*, \chi^k(g)=(\chi^k(g))^*$. If they are linearly independent, we deal with then cases (b, c) they transform according to joint degenerate reps $D^{\vec{k}}\oplus(D^{\vec{k}})^*$. We have tested the DVirrps of Si and Ge by means of Eqs. (4), (5). Most of the reps are of the form b and c cases. In here, we consider DVirrps regarded to edge band optical radiative transitions involving following reps: $\Gamma_{6\pm,7\pm,8\pm}$ (b) and $L_{4\pm,\ 5\pm,\ 6\pm}$, (c). According the TRS theory these states suppose to transform according to joint irrps. These states with Γ_{8+} (maximum of the VB) and L_{6+} (minimum of CB) symmetries transform now according to $\Gamma^{VB}_{8+}\oplus(\Gamma^{VB}_{8+})^*$, $L^{CB}_{6+}\oplus(L^{CB}_{6+})^*$ and $\Gamma^{CB}_{7-}\oplus(\Gamma^{CB}_{7})^*$ respectively. That is an essential modification of assignment, which results in extra degeneracy. This effect is rather seldom discussed in the literature. In Section 2.2 we discuss the optical selection rules for Ge and Si in the absence of TRS. In the presence of TRS these selection rules become: (TRS-KP)$=[\Gamma^{VB}_{8+}\oplus(\Gamma^{VB}_{8+})^*]\otimes[\Gamma^{CB}_{7-}\oplus(\Gamma^{CB}_{7-})^*]=\Gamma^{VB}_{8+}\otimes\Gamma^{CB}_{7-}\oplus\Gamma^{VB}_{8+}\otimes(\Gamma^{CB}_{7-})^*\oplus(\Gamma^{VB}_{8+})^*\otimes\Gamma^{CB}_{7-}\oplus\Gamma^{VB}_{8+}{}^*\otimes(\Gamma^{CB}_{7-})^*$. But $\Gamma^{VB}_{8+}\otimes\Gamma^{CB}_{7-}=\Gamma_{3-}\oplus\Gamma_{4-}\oplus\Gamma_{5-}$. Clearly, in this complex KP (TRS-KP) the symmetry of the perturbation Γ_{4-} (incident light) is contained. Therefore the triple KP: $[\Gamma^{VB}_{8+}\oplus(\Gamma^{VB}_{8+})^*]\otimes\Gamma_{4-}\otimes[\Gamma^{CB}_{7-}\oplus(\Gamma^{CB}_{7-})^*]$ contains identity rep Γ_1. Consequently, the direct radiative transition is allowed. Further evaluation of the TRS-KP yields: $4\Gamma_{3-}\oplus4\Gamma_{4-}\oplus4\Gamma_{5-}$. In here it has to be stressed out that TRS does not change the SRs in the absence of TRS. It only introduces more states of the same symmetry (Γ_{3-}, Γ_{4-}, Γ_{5-}). Similarly, for indirect transitions the selection rules are $[\Gamma^{VB}_{8+}\oplus(\Gamma^{VB}_{8+})^*]\otimes[L^{CB}_{6+}\oplus(L^{CB}_{6+})^*]=4\Gamma_{1+}\oplus4\Gamma_{2+}\oplus4(3\Gamma_{3+})$ [5]. In this KP the allowed symmetries of the phonons ($L_{1+,2+,3+}$) are contained. Therefore, the indirect transitions are allowed. And due to the TRS the number of different states of the same symmetry increases. Each basis will be a linear combination of the complex KP basis. These linear combinations can be obtained by Clebsch Gordon Coefficients method.

3. Conclusion

The inclusion of TRS does not affect the vibrational states in Si and Ge. The most pronounced phonons are not TRS degenerate.

Table 1 list some multiphonon selection rules regarded to phonons originating from high symmetry lines. They have appreciable impact on phonon density of states.

The optical selection rules in the presence of TRS are the same as in the absence of TRS. The only effect of the inclusion of TRS is an increase in the number of state with the same symmetries.

Experimentally, the observation (or not) of “extra” splitting of spectral degenerate terms will verify the existence of more electronic states.

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