Scattering tensors for Si and Ge with O_h^7 symmetry

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Keywords: First-order Raman scattering tensors in Si and Ge, Kronecker product, Clebsch-Gordan coefficients.

Abstract

The scattering tensors are of great importance in the interpretation of Raman scattering spectra. Using Birman's method we have calculated the Clebsch-Gordan coefficients (CGC's) for the first-order Raman scattering tensors in Si and Ge with O_h^7 symmetry. The matrix elements of the scattering tensors are the linear combinations of the CGC's.

1 Introduction

The study of scattering processes involving phonons provides valuable informations about various properties in semiconductors. In these materials the collective excitations are lattice vibrations, such as optical and acoustic phonons. Si and Ge are semiconductors of space group symmetry O_h^7 with relative small energy gap ($E_g \simeq 1.11$ eV for Si and $E_g \simeq 0.67$eV for Ge) and easily doped with resulting changes of electron density. The plasmas waves in the electron gas interact with incident light coupling phonons and plasmons. Scattering processes can occur at high symmetry points due to the interaction of carriers with phonons, impurities and so on. Lax and Hopfield [1] and Birman et al [2] have established the selection rules for direct and indirect transitions in Si and Ge. Away from the Brilloiun zone center the phonons participating in the Raman scattering processes are second order and are related to first-order Raman scattering processes. Only excitations having definite symmetry are allowed to participate in the first order Raman scattering [3]. The aim of this work is to calculate the CGC's for the first-order Raman scattering tensors for interaction involving photons with quasiparticles (one-phonon excitations) in Si and Ge. The organization of the paper is as follows. The first section introduces the paper with an overview of the interaction between the incident light and the phonons resulting in the scattering processes in materials. In the second section we give a summary of the theory of Raman scattering tensors enhanced by the calculations. In section three we present the results of the first-

order Raman scattering tensors arising from our calculations CGC's. We conclude the paper with a brief summary followed by the reference.

2 The summary of the theory of Raman scattering tensors

The states of quasiparticles such as phonons, plasmons, polarons, polaritons, excitons etc... are classified according to irreducible representations (irreps) of the space symmetry group. The interactions of particles and/or quasiparticles are represented by the Kronecker product (KP) of irreducible representations of the corresponding factor group $(G_0^{\mathbf{k}})/T$. The CGC's are matrix elements that diagonalize the KP of relevant irreps involved in the scattering processes.
The symmetry of a photon state is Γ_{4-} with this labelling taken from [4]. The KP of phonons states should contain the symmetry of the perturbing agent. At $\mathbf{k} = 0$ the long-wavelength , the modes originating from the zone center are of Γ symmetry . In Si and Ge the vector representation is Γ_{4-}. For Raman scattering the allowed phonons are contained in the symmetrized square of the Kronecker product of vector representation.

$$[\Gamma_{4-} \otimes \Gamma_{4-}]_2 \cong \Gamma_{1+} + \Gamma_{3+} + \Gamma_{5+} \tag{1}$$

The CGC's U matrix brings the above KP to the blocks diagonal form:

$$U^{-1} [\Gamma_{4-} \otimes \Gamma_{4-}]_2 U = \Gamma_{1+} + \Gamma_{3+} + \Gamma_{5+} \tag{2}$$

If the unit polarization vector of the incident radiation is denoted $\hat{\varepsilon}_1$ with Cartesian coordinates $\varepsilon_{1\beta}(\beta$ = x,y,z) and the unit polarization vector of the scattered radiation is denoted $\hat{\varepsilon}_2$ with Cartesian coordinates $\varepsilon_{2\alpha}$ (α = x,y,z), the intensity of the scattered light polarized in the direction α for incident light polarized in the direction β is [5]:

$$C|\varepsilon_{2\alpha} P\alpha\beta \varepsilon_{1\beta}|^2 \tag{3}$$

where $P_{\alpha\beta}$ is the scattering tensor see Eq.(4) as well, and C are the constants. The Raman scattering tensor operator is expanded in terms of the normal coordinates of the lattice Q_σ^j. The coefficients of the linear terms in the expansion Q_σ^j in Eq.(4) correspond to one-phonon scattering, in other words, the first-order Raman scattering tensor [5].

$$P_{\alpha\beta}(\vec{R}) = P_{\alpha\beta}^{(0)}(\vec{R}^0) + \sum_{j\sigma} P_{\alpha\beta}^{(1)}(\vec{R}^0; j\sigma) Q_\sigma^j + ... \tag{4}$$

where the $j\sigma$ indices are used to specify the symmetry species of phonon. The U matrix is obtained from [6]:

$$U^{\Gamma_{4-}\Gamma_{4-},l''}_{aa',a''} U^{\Gamma_{4-}\Gamma_{4-},l''*}_{\bar{a}\bar{a}'\bar{a}''} = \frac{dim(l'')}{2g} \sum_R [(\Gamma_{4-})_{aa'}(\Gamma_{4-})_{\bar{a}\bar{a}'} + (\Gamma_{4-})_{\bar{a}a'}(\Gamma_{4-})_{a\bar{a}'}] .\Gamma^{l''*}_{a''\bar{a}''} \quad (5)$$

where the irreps l'' are $\Gamma_{1+}, \Gamma_{3+}, \Gamma_{5+}$.

3 Results and discussion

The mathematical theory of CGC's has been developed by Berenson and Birman [7] who calculated the CGC's for Diamond (O_h^7) and rocksalt (O_h^5)[8], Kunert and Suffczynski [9, 10] developed the theory of the CGC's related to the wave vector selection rules in terms of block structures. The Raman scattering tensors in cubic Cu_2O (O_h^4) were analysed by Birman [11], Kunert et al. computed the CGC's for scattering tensors in ZnO and other wurtzite semiconductors [14]. Finally, Berenson [13] discussed the scattering tensors for crystals limited to the point groups T_d and C_{6v}. However, the first-order Raman scattering tensors for Si and Ge space groups have not been studied up to now.
In this paper, we have used the Eq.(5) to calculate and tabulate the CGC's for first-order Raman scattering tensors. Using these CGC's for symmetrized square of vector representation Γ_{4-} of Si and Ge space groups, we have constructed the first-order Raman scattering tensors in the form:

$$P_{\alpha\beta}(\Gamma) = \begin{pmatrix} xx & xy & xz \\ yx & yy & yz \\ zx & zy & zz \end{pmatrix} \quad (6)$$

The elements of the First-order Raman scattering tensors are comparable to the values found in the literature[12]. The elements of the first-Raman scattering tensors for Γ_3 tabulated by Loudon for point groups don't contain the phases $w = -\frac{1}{2} + i\frac{\sqrt{3}}{2}$ and $w*$. In our case, the space groups studied contain the phases at Γ point resulting in presence of the phases for the first-order Raman scattering tensor for Γ_3 irrep.

From our table, we have derived the first-order Raman scattering ten-

Table 1: The CGC's for the U matrix: $a = \frac{1}{\sqrt{2}}, b = \frac{1}{\sqrt{3}}$, and $w = -\frac{1}{2} + i\frac{\sqrt{3}}{2}$.

$[\Gamma_{4-} \otimes \Gamma_{4-}]_2 \cong$	Γ_{1+} +	Γ_{3+}		+	Γ_{5+}	
xx	b	b	b	0	0	0
xy	0	0	0	0	0	a
xz	0	0	0	0	a	0
yx	0	0	0	0	0	a
yy	b	w^* b	wb	0	0	0
yz	0	0	0	a	0	0
zx	0	0	0	0	a	0
zy	0	0	0	a	0	0
zz	b	wb	w^* b	0	0	0

sors resulting from the linear combinations of CGC's tabulated.

$$P_{\alpha\beta}(\Gamma_{1+}) = \begin{pmatrix} b & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & b \end{pmatrix}, P_{\alpha\beta}(\Gamma^1_{3+}) = \begin{pmatrix} b & 0 & 0 \\ 0 & w^*b & 0 \\ 0 & 0 & wb \end{pmatrix}, P_{\alpha\beta}(\Gamma^2_{3+}) = \begin{pmatrix} b & 0 & 0 \\ 0 & wb & 0 \\ 0 & 0 & w^*b \end{pmatrix},$$

$$P_{\alpha\beta}(\Gamma^1_{5+}) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & a \\ 0 & a & 0 \end{pmatrix}, P_{\alpha\beta}(\Gamma^2_{5+}) = \begin{pmatrix} 0 & 0 & a \\ 0 & 0 & 0 \\ a & 0 & 0 \end{pmatrix}, P_{\alpha\beta}(\Gamma^3_{5+}) = \begin{pmatrix} 0 & a & 0 \\ a & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

4 Conclusion

In summary, we have calculated the CGC's matrix elements of $[\Gamma_4 \otimes \Gamma_4]_2$ for Si and Ge. We have studied the first-order Raman scattering tensors in Si and Ge by means of CGC's. The CGC's are also used to estimate the energy of the scattering tensor [14]. The linear combinations of these elements of the first-Raman scattering tensors are the elements of the Brillouin zone scattering not discussed here. The one-phonon involved in these scattering processes are determined by irreps contained in KP.

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