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Elementary excitations in Si, Ge, and diamond time reversal affected

H.W. Kunert [a], A.G.J. Machatine [a,*], J.B. Malherbe [a], J. Barnas [b], A. Hoffmann [c], M.R. Wagner [c]

[a] Department of Physics, University of Pretoria, 0002 Pretoria, South Africa
[b] Department of Physics, Adam Mickiewicz University, ul. Umultowska 85, 61-614 Poznan, Poland
[c] Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergerstr. 36 10-623, Germany

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ABSTRACT

The Space Symmetry and the Time Reversal Symmetry of vibrational modes in Si, Ge and diamond are investigated. Using Space Symmetry we have derived the Lattice Mode Representation. Reducing it onto phonon species we obtain the symmetry allowed phonons and their degeneracies. Using reality test for irreducible representations according to those the phonons are classified we determine which modes are Time Reversal affected. Comparison with experimental data obtained by neutron scattering is made. The effect of Time Reversal Symmetry on electrons in the conduction band and holes in the valence band as well as on excitons is briefly discussed.

1. Introduction

The lattice dynamics of materials having the diamond structure have been subject of much experimental and theoretical investigation. The phonon spectra of diamond, silicon, and germanium have all been investigated by inelastic neutron, X-ray, and Raman (RS) scattering and also by infrared absorption (IR). Theory of IR and RS processes and group theoretical selection rules in diamond has been studied by Birman [1]. Selection rules for intervalley scattering for Ge and Si have been investigated by Lax and Hopfield [2]. Multiphonon processes in diamond structure were also investigated by several authors [3–7] and references therein. In here we use the standard method of placing displacement vectors upon each ion in the unit cell at $\mathbf{k}=0$, to obtain the 6×6 Lattice Mode Representation (LMR). The LMR contains two allowed symmetry modes: $\Gamma_{15}$and $\Gamma_{25}$for diamond, Si and Ge. The detailed derivation of LMR will be given elsewhere. Using compatibility relations over the entire Brillouin Zone (BZ) we obtain the symmetry allowed modes originating from high symmetry point and lines in these compounds. Our results are in agreement with theoretical and experimental data published in many papers and books. The assignment of phonons classified by real representations (RRs) follows from the LMR. However, some irrps of diamond (O_h^7) are complex. Consequently, we must consider the effect of Time Reversal Symmetry. Birman [8] and Bradley–Cracknell [9] hereafter as BC considered the effect of Time Reversal Symmetry (TRS) on X and L vibrational modes in diamond. In here we analyze the TRS impact on phonons states and on other quasi-particles like electrons, holes, excitons, plasmons, etc. The analysis involves group theoretical method. In the next section we recall the necessary theory of the TRS and apply to vibrational modes in Si, Ge, and diamond. In Section 2 we discuss the effect of TRS on phonon dispersion curves obtained experimentally. In Appendix, we provide some examples of detailed calculations on reality of irreducible representations (irrps). In Appendix are briefly reported the effect of TRS on electrons, holes, and excitons.

2. Degeneracy of spin-less vibrational states in crystals due to the Time Reversal Symmetry

When a specimen is neither subject to external magnetic field nor will exhibit spontaneous magnetic ordering, the Hamiltonian is invariant under the operation of the TR. The operator of TR, K takes eigenfunction Ψ of the Hamiltonian into a new complex function Ψ^*, $K\Psi=\Psi^*$ which satisfies the same equation as Ψ. In other words the inclusion of TRS may lead to an extra degeneracy of eigenfunctions (states) in addition to degeneracy resulting from dimensions of irrps of $D^{\mathbf{k}}$ of a space group of a crystal Space Symmetry $G^{\mathbf{k}}$ where $\boldsymbol{k}$ runs over the entire Brillouin Zone (BZ), for diamond see figure 3.14 in [9]. The Bloch functions $\Psi_{\mathbf{k}}(\boldsymbol{r})=u_{\mathbf{k}}(\boldsymbol{r})\ \exp(i\mathbf{k}\cdot\boldsymbol{r})$ subject to TR operator becomes $\Psi^*_{\mathbf{k}}(\boldsymbol{r})=u^*_{\mathbf{k}}\exp(i(-\mathbf{k}\cdot\boldsymbol{r}))$. Clearly, we deal now with two sets of functions (Ψ, Ψ^*) those are eigenfunctions of a given Hamiltonian. Consequently, the space group $G^{\mathbf{k}}$ has been enlarged twice in the number of symmetry elements by the time-inversion symmetry operator K. It means that all the symmetry operators $\{\boldsymbol{g}|\boldsymbol{t}\}$ must be multiplied by K. The new group becomes antiunitary and the irrps of the group are $\boldsymbol{D^k}\oplus(\boldsymbol{D^k})^*$ whenΨ and Ψ^* are linearly independent. Clearly, the degeneracy of these states is increased and they are now classified according to joint irrps $\boldsymbol{D^k}\oplus(\boldsymbol{D^k})^*$. This affects many phenomena. It will increase the dimension of dynamical matrices for phonon dispersion curves calculations, it will change the optical selection rules, scattering tensors, etc. In turn it means when an irrp of a space group is complex the TRS must be considered. It is therefore of

* Corresponding author.
E-mail address: augusto.machatine@up.ac.za (A.G.J. Machatine).

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importance to find out which irrps of a crystal are complex. Fröbenius and Schur [10] derived a criterion on reality of irrps. The tables of characters of irrps of 230 space groups are available [11,12]; thereafter referred as ML and CDML, respectively. The reality test has also been analyzed by Bradley and Cracknell [9]. They used their own derived irrps of space groups. In terms of BC and CDML notation we write the reality test as

$$\frac{f}{h}\sum_{R_\alpha} \chi_j^{\boldsymbol{k}}\left(\{R_\alpha|v_\alpha\}^2\right) = +1(\mathrm{a}), \quad 0\,(\mathrm{b}), \quad -1(\mathrm{c}) \tag{1}$$

where $\chi_j^{\mathbf{k}}$ is the character of the small irrp of $G^{\mathbf{k}}/T$, and the sum is restricted to those coset representative of $\{R_\alpha|\upsilon_\alpha\}$ of $G^{\mathbf{k}}$ with respect to T (group of pure translations) whose rotational parts send $\boldsymbol{k}$ into a vector equivalent to $-\boldsymbol{k}$. And f/h is the number of elements of $G^{\mathbf{k}}$ group.

$$R_\alpha \boldsymbol{k} = -\boldsymbol{k} + n_1\boldsymbol{b}_1 + \mathrm{n}_2\boldsymbol{b}_2 + \mathrm{n}_3\boldsymbol{b}_3 \tag{2}$$

The usefulness of the reality test of a representation lies in determining whether or not extra degeneracy occur if the crystal described by the space group also possesses time-inversion symmetry. The relation between the reality of a rep and these extra degeneracies followed from testing Eq. (1), is:

Single valued representations		Double valued representations	
Reality	Degeneracy	Reality	Degeneracy
1	a ($\sum\to+1$)	1	b ($\sum\to-1$)
2	b ($\sum\to-1$)	2	a ($\sum\to+1$)
3	c ($\sum\to0$)	3	c ($\sum\to0$)

(a) There is no change in the degeneracy of E($\boldsymbol{k}$)
(b) The degeneracy of E($\boldsymbol{k}$) doubles, that is two different energy levels, both described by the same rep become degenerate
(c) The degeneracy of E($\boldsymbol{k}$) becomes doubled, but unlike (b), two different (in-equivalent) reps become degenerate
(d) When $+\boldsymbol{k}$ and $-\boldsymbol{k}$ are not in the same star, the spectrum of the eigenvalues at $-\boldsymbol{k}$ becomes identical with the spectrum of the eigenvalues at $+\boldsymbol{k}$.

In other words, where there is no symmetry element in the space group that transforms $+\boldsymbol{k}$ into $-\boldsymbol{k}$ the addition of the time-inversion symmetry produces a type $(x)\to$(d) degeneracy. In this case the symbol (x) is used in place of the reality 1, 2, or 3. Using the CDML Tables and Eqs. (1), (2) we have investigated all high symmetry points and lines in diamond. We did not find the x type degeneracy in compounds of diamond structure, (see Table 1). In Appendix we give some instances of detailed calculations. Since in the early literature the irrps of O_h^7space group were labelled according to Bouckaert Smoluchowski Wigner (BSW) [13] in the determination of diamond, Si and Ge phonon dispersion curve we give the correspondence of irrps labels in Table 2.

Table 1
Space group number: 227

Points and lines	Coordinates	SV representations	BC [9]	Birman [8]	This paper
Γ	(0,0,0)	$\Gamma_{1\pm,2\pm,3\pm,4\pm,5\pm}$	a	–	a
X	$(\frac{1}{2},0,\frac{1}{2})$	$X_{1,2,3,4}(2)$ R-Reps	c	a	a
L	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$L_{1\pm,2\pm}(1)$, $L_{3\pm}(2)$ R-Reps	c	–	a
W	$(\frac{1}{2},\frac{1}{4},\frac{3}{4})$	$W_{1,2}(2)$ C-Reps	b	a	a
Δ	$(\alpha,0,\alpha)$	$\Delta_{1,2,3,4}(1)$, $\Delta_5(2)$ C-Reps	b	b	a
Λ	(α,α,α)	$\Lambda_{1,2}(1)$, $\Lambda_3(2)$ R-Reps	a	–	a
Σ	$(\alpha,\alpha,2\alpha)$	$\Sigma_{1,2,3,4}(1)$ C-Reps	c	–	a
Q	$(\frac{1}{2},\frac{1}{4}+\alpha,\frac{3}{4}+\alpha)$	$Q_{1,2}(1)$ R-Reps	c	–	a
S	$(\frac{1}{2}+\alpha,2\alpha,\frac{1}{2}+\alpha)$	$S_{1,2,3,4}(1)$ R-Reps	c	–	c
A	$(\alpha,-\alpha+\beta,\beta)$	$A_{1,2}(1)$ C-Reps	–	–	c
$Z=V$	$(\frac{1}{2},\alpha,\frac{1}{2}+\alpha)$	$Z_1=V_1(2)$ R-Reps	a	–	a

Fd3m, $O_h^7$for diamond C, Ge and Si.
Time Reversal Symmetry type of irreducible representation.

Table 2
Table of correspondence of labeling of irreducible representation at point Γ ($\boldsymbol{k}$=0), for space group O_h^7diamond, Si and Ge

CDML[1]	Miller, Love[2]	Zak, Casher[2]	Kovalev[2]	BC[2]	Elliot[2]	BSW[2]
Γ_{1+}	GM1+	1	$\mathrm{T2005}_{\tau_1}$	A_{1g}	Γ_{+}	Γ_1
Γ_{2+}	GM2+	2	$\mathrm{T2005}_{\tau_2}$	A_{2g}	Γ_{2+}	Γ_2
Γ_{3+}	GM3+	3	$\mathrm{T2005}_{\tau_3}$	E_g	Γ_{12+}	Γ_{12}
Γ_{4+}	GM4+	5	$\mathrm{T2005}_{\tau_5}$	T_{1g}	Γ_{15+}	$\Gamma_{15'}$
Γ_{5+}	GM5+	4	$\mathrm{T2005}_{\tau_4}$	T_{2g}	Γ_{25+}	$\Gamma_{25'}$
Γ_{1-}	GM1−	6	$\mathrm{T2005}_{\tau_6}$	A_{1u}	Γ_{1-}	$\Gamma_{1'}$
Γ_{2-}	GM2−	7	$\mathrm{T2005}_{\tau_7}$	A_{2u}	Γ_{2-}	$\Gamma_{2'}$
Γ_{3-}	GM3−	8	$\mathrm{T2005}_{\tau_8}$	E_u	Γ_{12-}	$\Gamma_{12'}$
Γ_{4-}	GM4−	10	$\mathrm{T2005}_{\tau_{10}}$	T_{1u}	Γ_{15-}	Γ_{15}
Γ_{5-}	GM5−	9	$\mathrm{T2005}_{\tau_9}$	T_{2u}	Γ_{25-}	Γ_{25}
Γ_{6+}	GM6+	$\bar{1}$	$\mathrm{P205}_{\pi_2}$	$\bar{E}_{1g}$	Γ_{6+}	
Γ_{7+}	GM7+	$\bar{2}$	$\mathrm{P205}_{\pi_1}$	$\bar{E}_{2g}$	Γ_{7+}	
Γ_{8+}	GM8+	$\bar{3}$	$\mathrm{P205}_{\pi_3}$	$\bar{F}_g$	Γ_{8+}	
Γ_{6-}	GM6−	$\bar{4}$	$\mathrm{P205}_{\pi_4}$	$\bar{E}_{1u}$	Γ_{6-}	
Γ_{7-}	GM7−	$\bar{5}$	$\mathrm{P205}_{\pi_5}$	$\bar{E}_{2u}$	Γ_{7-}	
Γ_{8-}	GM8−	$\bar{6}$	$\mathrm{P205}_{\pi_6}$	$\bar{F}_u$	Γ_{8-}	

References for Table 2 [1] A.P. Cracknell, B.L. Davis, S.C. Miller and W. F. Love, Kronecker Product Tables, Vol. 1–4, IFI/Plenum Press, New York, Washinton, London, 1979.[2] N. Houng, P. Tien, H. Kunert and Suffczynski, Journal de Physique, Tome 38, Janvier 1977, Page 51.

3. Degeneracy of quasi-particles with spin due to time-inversion symmetry

The states of spin-less quasi-particles like vibrational modes are classified according to the single valued representation (SVRs). However, the TRS may also affect the states of quasi-particles that carry spin, like electrons, holes, ions, and others. Therefore, it is often necessary to take into account the existence of the spin of an electron and hole due to the introduction of relativistic effects into electron and hole band structure determination or inclusion spin–orbit and spin–spin interaction in the crystal field theory. Inclusion of spin results into a double space group described now by SVRs and double valued reps (DVRs). At $\boldsymbol{k}$=0 the diamond double group has got $\Gamma_{1\pm,2\pm,3\pm,4\pm,5\pm}$ SVRs and $\Gamma_{6\pm,7\pm,8\pm}$ DVRs CDML [12] notation (see Table 2). At other high symmetry point and lines the DVRs are: X_5, $L_{4\pm,5\pm,6\pm}$, $W_{3,4,5,6,7}$, $\Delta_{6,7}$, $\Lambda_{4,5,6}$, Σ_5, S_5, and $Z=V_{2,3,4,5}$. The reality test for DVRs yields: $\Gamma_{6\pm,7\pm,8\pm}$(c), X_5(a), $L_{4\pm,5\pm}$(b), $L_{6\pm}$(c), $\Delta_{6,7}$, (b). The letters in brackets indicate the type of degeneracy. The electronic band structure of Si, Ge and diamond must be described by DVRs. The minimum of the conduction band is at $\Gamma_{7-}$and the maximum of the valence band at (see figure 6.13 P. Yu and M. Cardona, p. 268 [14]). The states of electrons and holes are classified now according to joint DVRs:

$\Gamma_{6+}\oplus\Gamma_{6+}^*$, $\Gamma_{6-}\oplus\Gamma_{6-}^*$, $\Gamma_{7+}\oplus\Gamma_{7+}^*\Gamma_{7-}\oplus\Gamma_{7-}^*$, $\Delta_7\oplus\Delta_7^*$. When spin excluded the bands edge transitions in diamond are $\Gamma_{25'}\to\Delta_1$, $\Gamma_{25'}\to\Gamma_{15'}$, $X_4\to X_1$, $L_{3'}\to L_{1'}$[15]. Inclusion of spin leads to the following band edge assignments: the maximum of the valence band (VB) is at $\Gamma_{8+}\oplus(\Gamma_{8+})^*$, and the minimum of the conduction (CB) band at $\Gamma_{7-}\oplus\Gamma_{7-}^*$, etc. It means, that the edge bands at $\boldsymbol{k}$=0 are TRS subject. The selection rules for direct and indirect radiative transitions will be now essentially affected by TRS. For example the edge transition $(\Gamma_{8+}\oplus(\Gamma_{8+})^*)^{\mathrm{VB}}\to(\Gamma_{7-}\oplus\Gamma_{7-})^*)^{\mathrm{CB}}$ will be allowed if Kronecker Product (KP) $(\Gamma_{8+}\oplus(\Gamma_{8+})^*)^{\mathrm{VB}}\otimes(\Gamma_{7-}\oplus\Gamma_{7-})^*)^{\mathrm{CB}}$ contains the symmetry of the perturbation under TRS [16]. In other words extra KPs, like $\Gamma_{8+}^*\otimes T_{7-}$ have to be evaluated. On the other hand, the symmetry of direct excitons in Ge is the product of CB and VB symmetries; due to the exchange interaction the exciton of symmetry $(\Gamma_{8+}\oplus(\Gamma_{8+})^*)^{\mathrm{VB}}\otimes(\Gamma_{7-}\oplus\Gamma_{7-})^*)^{\mathrm{CB}}$ splits onto: $4\Gamma_{3-}\oplus4\Gamma_{4-}\oplus4\Gamma_{5-}$. The

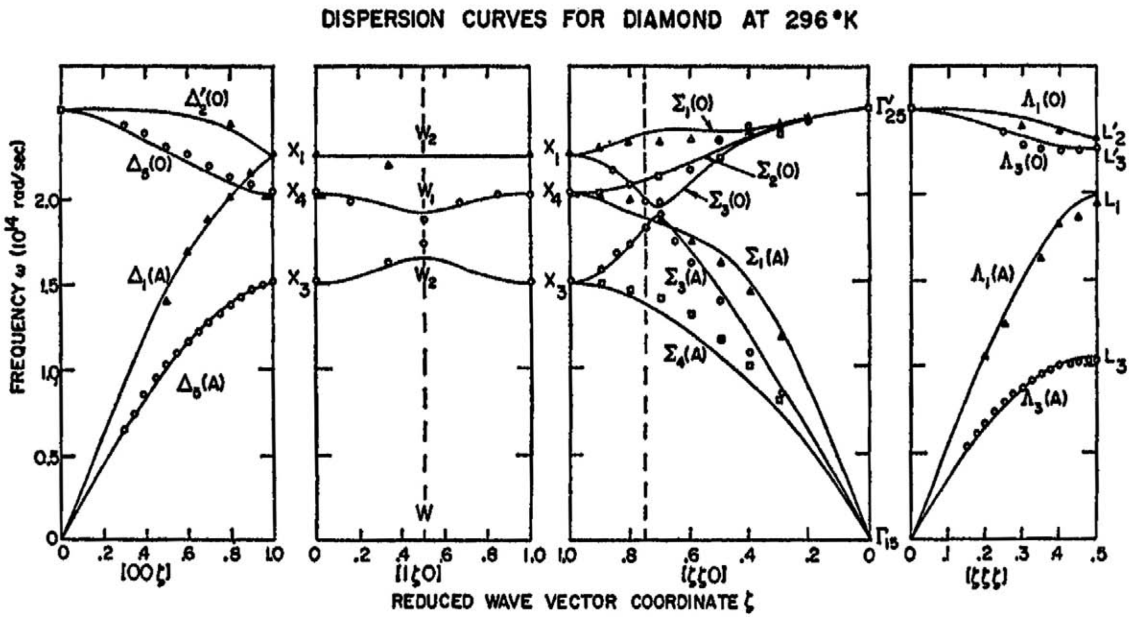

Fig. 1. The dispersion relation for the normal modes of vibration of diamond in the principal symmetry directions at 296°K. The full curves represent a shell-model fit to the data points. Branches and end points are labeled by the irreducible representations according to which the associated polarization vectors transform.

symmetry of perturbation (light) $\Gamma_{4-}$is contained in the KP decomposition. Therefore the radiative transition is allowed. The inclusion of TRS in the band structure is in terms of DV irrps and does not change the selection rules in the absence of TRS. It increases the number of allowed states. Consequently, the existence of TRS leads to the necessary modification of optical selection rules in crystals. In here we only briefly indicate the consequences of the TRS presence in crystals. The detailed discussion on optical selection rules due to TRS will be given elsewhere.

4. Discussion

From Table 1 follows that in diamond, Si and Ge all vibrational modes originating from high symmetry points, Γ, X, L and W are classified according to the real reps, case (a). Clearly, these phonons are not subject to TRS and there is no extra degeneracy. These features have already been long time ago approved by experimental data obtained by neutron scattering, infrared absorption, and X-ray spectroscopy [3]. We have calculated the compatibility relations starting from phonons at $\boldsymbol{k}=0$ obtained by LMR. Our results are in perfect agreement with the experimental data. For example, going from through Γ, Δ, Λ and Σ symmetry lines towards the X, L and K, respectively, we obtain high symmetry lines presented on Fig. 1 [3]. The most striking feature obtained by BC of X, L, and W phonons is their TRS extra degeneracies cases (b) and (c), see Table 1. Their results are in extreme contrast to experimental results. They used different coordinate systems, and therefore different non-primitive translations associated with the rotational symmetry operators. Birman [8] discussed the effect of TRS on X and W phonons. Regarding point X we are in a good agreement with Birman. The irrps of $G^{\mathbf{k}W}$, $W_{1,2}$are essentially complex. However, he proved that in spite of the appearance of complex number in the characters of W_1, W_2both reps are real. We have performed exact calculations based on Eqs. (1), (2) obtaining the same results. Concerning the high symmetry lines we have found that lines A and S phonons TRS influenced (case (c)).

5. Conclusion

In diamond structure most pronounced vibrational states do not experience extra degeneracy when TRS included. Only two modes A and S are TRS degenerate. Electronic band structure of Si and Ge experience extra degeneracy. Consequently, optical selection rules are supposed to be modified by the inclusion of TRS.

Appendix A

The numbers in brackets denote the dimensions of irrps. Points and lines are in $\mathbf{g}_1$, $\mathbf{g}_2$, $\mathbf{g}_3$ coordinates. Single Valued (SV) representations.

$(\mathbf{g}\|\boldsymbol{\tau})$	1	2.2	3.3	4.1	21	22.2	23.3	24.1	25	26.2	27.3	28.1	45	46.2	47.3	48.1
X_1	2	0	2	0	0	0	0	0	0	0	0	0	2	0	2	0
X_2	2	0	2	0	0	0	0	0	0	0	0	0	−2	0	−2	0
X_3	2	0	−2	0	0	0	0	0	0	0	0	0	0	0	0	0
X_4	2	0	−2	0	0	0	0	0	0	0	0	0	0	0	0	0
$\mathbf{g}^2$	1	1	1	1	1	$3.3t_0$	1	$3.3t_0$	1	1	1	1	1	$3.3t_0$	1	$3.3t_0$
$\{\mathbf{g}\|\boldsymbol{\tau}\}\exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}_0)$	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1
$X_{1,2}$	2	−2	2	−2	2	2×(−1)	2	2×(−1)	2	−2	2	−2	2	2×(−1)	2	2×(−1)
$X_{3,4}$	2	−2	2	−2	2	−2×(−1)	2	−2×(−1)	2	−2	2	−2	2	−2×(−1)	2	−2×(−1)

$$R=\frac{1}{|g|}\sum_{g}\chi\left(\{\mathbf{g}^2|\mathbf{g}\tau+\tau\}\right)=\frac{1}{|g|}\sum_{g}\chi\left(\{\mathbf{g}^2|\tau_g\}\exp(-i\mathbf{k}\ \cdot\mathbf{t}_0)\right)$$

The $X_{1,2}$are complex third kind, (c) case ($R=0$) and $X_{3,4}$are real first kind (a) case ($R=1$).

$L=(\frac{1}{2},\frac{1}{2},\frac{1}{2})$												
{**g**|000}	1	5	9	13	17	21	25	29	33	37	41	45
{$\mathbf{g}^2$|000}	1	9	5	1	1	1	1	9	5	1	1	1

$$R=\frac{1}{|g|}\sum_{g}\chi(\{\mathbf{g}^2|000\})=\frac{1}{12}(8\chi(1)+2\chi(5)+2\chi(9))$$

$\mathbf{g}^2$	1	5	9	R
$L_{1+,2+}$	1	1	1	1(a)
L_{3+}	2	−1	1	1(a)
$L_{1-,2-}$	1	1	−1	1(a)
L_{3-}	2	−1	−1	1(a)

All $L_{1\pm,2\pm,3\pm}$are real and summation is done for all the symmetry elements for $k_L=(\frac{1}{2},\frac{1}{2},\frac{1}{2})-(\mathbf{g}_1,\mathbf{g}_2,\mathbf{g}_3)=-\boldsymbol{k}_L$.
$W=(\frac{1}{2},\frac{1}{4},\frac{3}{4})$ Reality test. Matrices and characters of $\{\mathbf{g}|\boldsymbol{\tau}\}$ and $\{\mathbf{g}^2|\mathbf{g}\boldsymbol{\tau}+\boldsymbol{\tau}\}$.

$\{g\|\tau\}$	1	2.2	17	18. 2	27. 3	28.1	43.1	44.1
W_1	$\begin{matrix}1 & \\ & 1\end{matrix}$	$\begin{matrix}1 & \\ & -1\end{matrix}$	$\begin{matrix} & -1\\ -1 & \end{matrix}$	$\begin{matrix}1 & \\ & -1\end{matrix}$	$\begin{matrix} & i\\ -1 & \end{matrix}$	$\begin{matrix} & i\\ 1 & \end{matrix}$	$\begin{matrix}1 & \\ & i\end{matrix}$	$\begin{matrix}1 & \\ & -i\end{matrix}$
W_2	$\begin{matrix}1 & \\ & 1\end{matrix}$	$\begin{matrix}1 & \\ & -1\end{matrix}$	$\begin{matrix} & 1\\ 1 & \end{matrix}$	$\begin{matrix}1 & \\ & -1\end{matrix}$	$\begin{matrix} & i\\ -1 & \end{matrix}$	$\begin{matrix} & i\\ 1 & \end{matrix}$	$\begin{matrix}-1 & \\ & -i\end{matrix}$	$\begin{matrix}-1 & \\ & i\end{matrix}$

Characters of ($\boldsymbol{g}$)	1	2.2	17	18.2	27.3	28.1	43.1	44.1
W_1	2	0	0	0	0	0	A, V	A, V^*
W_2	2	0	0	0	0	0	A, V	$-A, V^*$
$\mathbf{g}^2$	1	1	1	1	1	1	$2.2t_0$	$2.2t_0$
g2 exp($4\pi i\mathbf{k}\cdot\boldsymbol{t}_0$)	1	1	1	1	$-i$	i	$-i$	i
$\chi(\{\mathbf{g}\|\boldsymbol{\tau}\}^2)$	2	2	2	2	$-2i$	$+2i$	$0\times(-i)$	$0\times(i)$

$A=\sqrt{2}$,$V=\exp(i4\pi)$, $V^*=\exp(-i4\pi)$

The summation over the elements of the space group yields $R=1$. Therefore the $W_1$and W_2 are of the first kind (a) real. The symmetry operators are labels are according to CDML [12].

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