# On the determination of 'effective charges' associated with local vibrational modes

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**Abstract.** The integrated intensities of the absorption lines due to local vibrational modes of defects of $T_d$ and $C_{3v}$ symmetry are calculated as a function of the parameter measuring the strength of the coupling between the mode and the electric field associated with the light beam. In the case of $C_{3v}$ symmetry defects, the derivation does not assume this parameter to be the same for the longitudinal and transverse modes. The model is applied to the centres resulting from the neutralization by hydrogen of shallow dopants in crystalline semiconductors.

## 1. Introduction

Infrared measurement of local vibrational modes (LVM) is one of the most powerful tools for the study of light impurities in solids. In particular, hydrogen is widely studied by this technique both in amorphous and crystalline semiconductors. Two basic pieces of physical information can be obtained from an LVM spectrum: the energies of the modes give access to the force constants of the modes whereas their integrated intensity should allow the electric dipole moment associated with each mode of vibration or the so called effective charge of the mode to be obtained. In order to obtain the latter, the standard formula (Newman 1973, Cardona 1983, Newman 1992a)

$$I = \int \alpha(\omega)\, \mathrm{d}\omega = \pi N \eta^2 / 2nc\epsilon_0 m_{\mathrm{imp}} \qquad (1)$$

(expressed in SI units) is used. In this formula, $N$ is the concentration of impurities, $\eta$ the effective charge of the impurity, $m_{\mathrm{imp}}$ its mass, $n$ the refractive index of the material, $\epsilon_0$ the permittivity of vacuum, $c$ the velocity of light and $\omega$ its angular frequency. $\eta$ is not only characteristic of the impurity, but also of its surrounding (Leigh and Szigeti 1967a, b, 1968).

(1) is valid for triply degenerate modes of vibration of an impurity at a lattice site having the cubic system symmetry ($T_d$ in the case of silicon or the most common III-V semiconductors). However, (1) is often used for local modes of vibration of centres having a symmetry lower than cubic (often $C_{3v}$ symmetry); moreover, (1) is used very differently in the numerous papers which use it in this case. Some authors consider that $I$ is the total integrated intensity of all the modes (longitudinal + transverse) associated with one bond (for instance Pajot *et al* 1988 or Bergman *et al* 1988)

whereas other authors consider that $I$ is the integrated intensity of one of the modes (longitudinal or transverse) associated with the bond (for instance Kozuch *et al* 1990 or Woodhouse *et al* 1991). The fact that the 'effective charge' can be very different for the longitudinal and transverse modes (Jones and Oberg 1991, Jones *et al* 1992) associated with the same bond also makes the use of (1) questionable in the case of low-symmetry centres. In order to try to clarify the determination of the effective charges associated with a vibrational mode and to allow a comparison between the experimental results and the calculated effective charges, this paper reports on a derivation of the integrated intensities of LVMs of $T_d$ and $C_{3v}$ symmetries.

## 2. Integrated intensities of complexes having $T_d$ symmetry

### 2.1. Derivation

We describe the considered complex by a cluster of $T_d$ symmetry; the number of modes associated with the complex depends on the size of the cluster and each mode will transform according to one of the representations of the $T_d$ group. In this group, the electric dipole moment transforms according to the $\Gamma_5$ representation. As $\Gamma_5$ is contained once only in the symmetric products $[\Gamma_4 \times \Gamma_4]_S$ and $[\Gamma_5 \times \Gamma_5]_S$, in first order only the $\Gamma_4$ and $\Gamma_5$ vibrational modes are infrared active. Both of these modes are three-dimensional. If, moreover, one considers only transitions from the ground state (which transforms according to the $\Gamma_1$ representation), only $\Gamma_5$ vibrational modes are infrared active. Therefore, the time dependent electric dipole Hamiltonian describing the interaction of light (characterized by an electric field $E(t)$ of amplitude $E_0$ and angular frequency $\omega$) with a $\Gamma_5$ three-dimensional mode described by its normal coordinates $Q_x$, $Q_y$ and $Q_z$ is:

$$\mathcal{H}(t) = a[Q_x E_x(t) + Q_y E_y(t) + Q_z E_z(t)]$$

where $E_x(t)$, $E_y(t)$ and $E_z(t)$ are the three components of $E(t)$. The constant $a$ measures the strength of coupling of the light to the LVM. As the normal coordinates have the dimension of a length multiplied by the square root of a mass, $a$ has the dimension of a charge divided by the square root of a mass. As is usually done, we can write $a = -\eta/\sqrt{\mu}$ where $\mu$ is the reduced mass of the mode and $\eta$ its effective charge. However, one should keep in mind that the coupling between the mode of vibration and the light does not depend on two parameters $\eta$ and $\mu$ but only one, $a$, which can be extracted from the experimental results.

If one writes $\mathcal{H}(t) = H \sin \omega t$ with

$$H = a(Q_x E_{0x} + Q_y E_{0y} + Q_z E_{0z})$$

where $E_{0x}$, $E_{0y}$ and $E_{0z}$ are the three components of the amplitude $E_0$ of the electric field associated with the light, the transition probability per unit time between the ground state and the first excited state is given by the Fermi golden rule:

$$p(\omega) = (\pi/2\hbar^2)(|\langle 1,0,0|H|0,0,0\rangle|^2 + |\langle 0,1,0|H|0,0,0\rangle|^2$$
$$+ |\langle 0,0,1|H|0,0,0\rangle|^2)\delta(\omega - \omega_0)$$

where $|n_x, n_y, n_z\rangle$ denotes an eigenstate of the mode of angular frequency $\omega_0$. The necessary non-zero matrix elements are

$$\langle 1,0,0|Q_x|0,0,0\rangle = \langle 0,1,0|Q_y|0,0,0\rangle = \langle 0,0,1|Q_z|0,0,0\rangle = \sqrt{\hbar/2\omega_0}.$$

Therefore

$$p(\omega) = (\pi/2\hbar^2)(\hbar/2\omega_0)a^2(E_{0x}^2 + E_{0y}^2 + E_{0z}^2)\delta(\omega - \omega_0) = (\pi/4\hbar\omega_0)a^2 E_0^2 \delta(\omega - \omega_0).$$

In this expression, $E_0$ is the local electric field amplitude at the cluster.

The absorption cross section $\sigma(\omega)$ of the mode can be expressed as the ratio between the energy absorbed per unit time and the mean value of the electromagnetic energy flux:

$$\sigma(\omega) = [p(\omega)\hbar\omega / \tfrac{1}{2}nc\epsilon_0 E_0^2]\delta(\omega - \omega_0).$$

In this expression, $E_0$ is the average amplitude of the electric field in the sample and we assume that it is the same as the local one at the defect.

In fact, the absorption is never a Dirac peak, but is broadened by homogeneous and inhomogeneous processes; it is therefore necessary to introduce a normalized distribution function centred at $\omega_0$ : $\rho(\omega - \omega_0)$. If one assumes the width of this distribution to be small compared with $\omega_0$ (which is well justified for light impurities in crystalline semiconductors) and if there are $N$ defects per unit volume, the absorption coefficient can be written:

$$\alpha(\omega) = (\pi N a^2 / 2nc\epsilon_0)\rho(\omega - \omega_0).$$

The integrated intensity $I$ is therefore given by

$$I = (\pi N a^2 / 2nc\epsilon_0) = (\pi N \eta^2 / 2nc\epsilon_0\mu).$$

## 2.2. Discussion

The expression we obtain is practically the same as (1). This is of course expected as our derivation is mainly based on symmetry arguments which are taken into account in (1). An alternative expression of $a$, better adapted for theoretical calculations, is given in the appendix. Our derivation demonstrates that the integrated intensity depends only on the coupling strength $a$. The effective charge and the reduced mass of the mode are not independently accessible from the experiment.

## 3. Integrated intensities of complexes having $C_{3v}$ symmetry

In this section, we shall extend the derivation of the previous section to centres of $C_{3v}$ symmetry. Such centres are quite common, for instance several hydrogen related defects in semiconductors have this symmetry locally. In this group, there are one- and two-dimensional modes of vibration. The one-dimensional ones correspond to longitudinal modes and the two-dimensional ones to transverse modes with respect to the trigonal axis.

We shall use the notations of Koster *et al* (1963) and call $z$ the trigonal axis and $x$ and $y$ two rectangular axes perpendicular to $z$.

The time dependent electric dipole Hamiltonians $\mathcal{H}_l(t)$ and $\mathcal{H}_t(t)$ describing the interaction of light (characterized by a linearly polarized electric field $E(t)$ of amplitude $E_0$ and angular frequency $\omega$) with a longitudinal mode (described by the normal coordinate $Q_z$) and a doubly degenerate transverse one (described by the normal coordinates $Q_x$ and $Q_y$) can be written:

$$\mathcal{H}_l(t) = a_1 Q_z E_z(t) = a_1 Q_z E_{0z} \sin \omega t$$

with $E_{0z} = E_0 \cos\theta$ where $\theta$ is the angle between the electric field of the light and the $z$ axis, and

$$\mathcal{H}_t(t) = a_t[Q_x E_x(t) + Q_y E_y(t)] = a_t(Q_x E_{0x} + Q_y E_{0y})\sin\omega t.$$

Using the same algebra, approximations and notations as in section 2, the integrated intensities $I_1$ and $I_t$ associated with the longitudinal and transverse modes are

$$I_1 = \pi N a_1^2 \langle\cos^2\theta\rangle/2nc\epsilon_0 = \pi N \eta_1^2 \langle\cos^2\theta\rangle/2nc\epsilon_0\mu_1$$

$$I_t = \pi N a_t^2 \langle\sin^2\theta\rangle/2nc\epsilon_0 = \pi N \eta_t^2 \langle\sin^2\theta\rangle/2nc\epsilon_0\mu_t$$

where $\langle\cos^2\theta\rangle$ and $\langle\sin^2\theta\rangle$ are the averages of $\cos^2\theta$ and $\sin^2\theta$ over all the defects responsible for the absorption line and $\eta_1$ and $\eta_t$ the effective charges associated with the longitudinal and transverse modes of effective masses $\mu_1$ and $\mu_t$.

A light impurity in a centre of $C_{3v}$ symmetry is associated with two LVMs having different frequencies: a longitudinal one and a transverse one. For a substitutional impurity in a crystal of $C_{3v}$ symmetry, all the defects have the same $z$ axis and it is not necessary to average $\cos^2\theta$ and $\sin^2\theta$; in this case, the electric dipole transitions are fully polarized (parallel to the trigonal axis for the longitudinal modes and perpendicular to it for the transverse modes). However, as we shall see in the next section, there are several cases where locally the symmetry of the clusters is trigonal even though the symmetry of the crystal is not trigonal; in such cases $\theta$ is not the same for all the defects, and average values of $\cos^2\theta$ and $\sin^2\theta$ on all the defect orientations have to be taken.

## 4. Applications to amorphous materials and to $C_{3v}$ centres in cubic crystals

In amorphous materials, there is short range order, but no long range order. In such a case, one can have a local $C_{3v}$ symmetry. Such a model is able to describe for instance the vibrations of Si–H or Si–H$_3$ centres in hydrogenated amorphous silicon (but not those of Si–H$_2$). In amorphous material, as there is no long range order, at the scale of the light beam (diameter $\simeq 1$ mm) in the infrared experiments, the orientation of the local $z$ axes of the complexes is randomly distributed in three-dimensional space and therefore $\langle\cos^2\theta\rangle = 1/3$ and $\langle\sin^2\theta\rangle = 2/3$.

Our model also describes for instance the centres resulting from the neutralization by hydrogen of shallow dopants in silicon and III–V semiconductors (Stavola and Pearton 1991, Chevallier *et al* 1991, Pearton *et al* 1992). In these cases, the bonds involving hydrogen are oriented along the trigonal axes of the lattice. At equilibrium, there is an equal distribution of the bond orientations among the four trigonal axes. In such a case, whatever the light electric field orientation, $\langle\cos^2\theta\rangle = 1/3$ and $\langle\sin^2\theta\rangle = 2/3$ (which means that the transitions are unpolarized). These expressions are not appropriate for samples submitted to non-random stresses such as applied uniaxial stress or stresses due to lattice mismatch in heteroepitaxies.

Therefore, in both of the cases considered:

$$I_1 = \pi N a_1^2/6nc\epsilon_0 \tag{2}$$

$$I_t = \pi N a_t^2/3nc\epsilon_0. \tag{3}$$

One notes that if the coupling strengths $a_1$ and $a_t$ associated with the two modes involving one bond are identical, then $I_1 + I_t$ is given by (1). Therefore, in the two cases considered, (1) cannot be applied to the integrated intensity associated with only one mode (longitudinal or transverse).

## 5. Coupling factors of the centres resulting from the neutralization by hydrogen of shallow dopants in crystalline semiconductors

Experimental results available for the centres resulting from the neutralization of shallow acceptors in crystalline semiconductors concern only the longitudinal mode of vibration of the complex. Using the formula (2) derived in the previous section, one obtains the longitudinal coupling coefficients $a_l$ which are quoted in table 1. The refractive indices which have been used are $n = 3.4$ for silicon, $n = 3.3$ for GaAs, $n = 3.1$ for InP and $n = 2.9$ for AlAs. One notes that the values derived from the experiments for the C–H complex in GaAs are in quite good agreement with the one obtained from first principle calculations: $a_l = 0.96e/\sqrt{m_H}$ (Jones and Oberg 1991, Jones *et al* 1992).

**Table 1.** Longitudinal coupling factor $a_l$ of the complexes resulting from the neutralization of shallow acceptors in crystalline semiconductors by $X$ = hydrogen or deuterium. $a_l$ is expressed in units of elementary charge × (X atom mass)$^{-1/2}$. The $a_l$ values are obtained from (2) using the experimental data given in the quoted references.

| Host | Complex | $|a_l|\sqrt{m_X}/e$ | Reference |
|------|---------|--------------------|-----------|
| Si | B$\cdots$H—Si | 2.7 | McQuaid *et al* (1991) |
| | | 2.9 | Veloarisoa *et al* (1992) |
| | Al$\cdots$H—Si | 3.3 | Stavola *et al* (1987) |
| | Ga$\cdots$H—Si | 5.0 | Stavola *et al* (1987) |
| GaAs | Be$\cdots$H—As | 1.1 | Nandhra *et al* (1988) |
| | Be$\cdots$D—As | 1.4 | Nandhra *et al* (1988) |
| | Zn$\cdots$H—As | 0.72 | Chevallier *et al* (1991) |
| | C$_{As}$—H$\cdots$Ga | 0.75 | Woodhouse *et al* (1991) |
| | | 1.1[a] | Veloarisoa *et al* (1992) |
| | | 0.8–1.1 | Newman (1992b) |
| InP | Zn$\cdots$H—P | 0.98 | Chevallier *et al* (1991) |

[a] This value assumes that all the hydrogen in the layers is involved in C$_{As}$–H complexes and that the different C$_{As}$–H stretching features have the same calibration factor.

For the centres resulting from the neutralization of shallow donors, both longitudinal and transverse local vibrational modes are observed. The coupling factors $a_l$ and $a_t$ derived from the experimental data using the formulae obtained in section 4 are given in table 2.

An interesting fact to be noted is that in the same host (silicon), and for LVMs governed by Si—H bonds, $|a_l|$ and $|a_t|$ are around $1e/\sqrt{m_H}$ for the complexes resulting from the neutralization of shallow donors (cf table 2) whereas $|a_l|$ is clearly larger than $1e/\sqrt{m_H}$ in the case of the complexes resulting from the neutralization of shallow acceptors (cf table 1). This is probably due to the different microscopic structure in the two cases, hydrogen being in a bond centred location in the acceptor related complexes and in an antibonding location in the donor related ones.

For the centres resulting from the acceptor neutralization, it becomes apparent from table 1 that $|a_l|$ is around $1e/\sqrt{m_H}$ in the case of III–V compounds whereas it is clearly larger in the case of silicon. In the case of neutralized donors, such a trend does not exist; moreover table 2 shows that $|a_l| > |a_t|$ for Si and AlAs whereas the reverse situation occurs for GaAs. Hence no clear trend appears and detailed

**Table 2.** Longitudinal and transverse coupling factors $a_l$ and $a_t$ of complexes resulting from the neutralization of shallow donors in crystalline semiconductors by X = hydrogen or deuterium. $a_l$ and $a_t$ are expressed in units of elementary charge × (X atom mass)$^{-1/2}$. The $a_l$ and $a_t$ values are obtained from (2) and (3) using the experimental data given in the quoted references.

| Host | Complex | $|a_l|\sqrt{m_X}/e$ | $|a_t|\sqrt{m_X}/e$ | Reference |
|------|---------|--------------------|--------------------|-----------|
| Si | P$\cdots$Si—H | 0.92 | 0.89 | Bergman *et al* (1988) |
| | As$\cdots$Si—H | 1.3 | 1.2 | Bergman *et al* (1988) |
| | Sb$\cdots$Si—H | 0.97 | 0.86 | Bergman *et al* (1988) |
| GaAs | As$\cdots$Si$_{Ga}$—H | 0.83 | 1.0 | Pajot *et al* (1988) |
| | | 0.93 | 1.1 | Tuncel *et al* (1992) |
| | As$\cdots$Si$_{Ga}$—D | 0.74 | 0.91 | Pajot *et al* (1988) |
| AlAs | As$\cdots$Si$_{Al}$—H | 2.4 | 1.6 | Tuncel *et al* (1992) |

calculations such as those of Jones *et al* (1991, 1992) are probably necessary to explain the values given in tables 1 and 2. The analysis of the As$\cdots$Si$_{Al}$—H complex in AlAs (cf table 2) shows experimentally that $|a_l|$ and $|a_t|$ can be clearly different from each other.

The comparison of Be$\cdots$H—As and Be$\cdots$D—As complexes (cf table 1) on one hand, and of As$\cdots$Si$_{Ga}$—H and As$\cdots$Si$_{Ga}$—D complexes (cf table 2) in GaAs on the other, are of interest. The 'effective charges' have an essentially electronic origin and therefore should not depend upon the isotope. Therefore the differences between the coupling factors of pairs of complexes reflect the differences of their reduced mass. As the hydrogen and deuterium atoms are much lighter than the other atoms of the cluster, one is tempted to assume that the reduced mass of the cluster is equal to the hydrogen or deuterium mass; if this were correct, one should get the same numbers for the hydrogenated and deuterated related complexes (because of the different units used for the hydrogenated and deuterated complexes). The fact that this is not the case seems to provide evidence that the cluster reduced mass involves all the cluster atoms and not only the impurity one even in the case of very light impurities. As the determination of the coupling factors requires the measurement of the complex concentrations which is very delicate, one could suspect the uncertainties on these measurements to be responsible for the differences discussed above.

However, the involvement of all the cluster atoms in the reduced mass even in the case of very light impurities is confirmed by the data of Bergman *et al* (1988) on donor-hydrogen and donor-deuterium complexes in silicon. Their data do not allow the determination of $a_l$ and $a_t$ for the deuterated complexes, but they provide their ratios which are given in table 3. These ratios are clearly different which shows that the ratios of the reduced masses $\mu_l/\mu_t$ are different for the hydrogenated and deuterated clusters. It is to be noted that each value given in table 3 comes from a single precise spectroscopic experiment and that the concentration of the complexes does not have to be known for obtaining these values; therefore these numbers are quite accurate.

These data therefore demonstrate another weakness of (1): the appearance of the impurity mass rather than the reduced mass of the cluster.

**Table 3.** $|a_t|/|a_l|$ ratios for the centres resulting from the neutralization of donors in silicon by hydrogen and deuterium. The experimental data are from Bergman *et al* (1988).

|            | H    | D   |
|------------|------|-----|
| P···Si—    | 0.97 | 1.1 |
| As···Si—   | 0.92 | 1.1 |
| Sb···Si—   | 0.89 | 1.1 |

## 6. Conclusion

In this paper, we have shown that the determination of the electric dipole moment associated with one local vibrational mode is not obvious and that some care has to be taken when trying to extract it from infrared absorption experiments. The experiment does not provide a direct value of the effective charge associated with the mode, but the ratio between the effective charge and the square root of the reduced mass of the mode. We suggest the $a$ parameters to be the appropriate ones to quote rather than the effective charges. The cases considered in this paper are simple ones involving complexes of $T_d$ or $C_{3v}$ local symmetry. The derivations can be easily extended to more complex centres such as Si–$H_2$ in amorphous silicon.

## Acknowledgments

## Appendix

In the body of the article we have mainly addressed the problem of the determination of the coupling strengths from the experiments. It is of course essential to determine the same quantities theoretically. In this appendix we give expressions of the coupling strengths more suitable for theoretical investigations.

The general Hamiltonian describing the electric dipole interaction of the cluster with the light is

$$\mathcal{H}(t) = -p \cdot E(t)$$

where $p$ is the total electric dipole moment of the cluster.

$p$ can be expanded in powers of the normal modes of the cluster. The static electric dipole moment does not induce any absorption. The Hamiltonians used in this article are limited to first order in the values of $Q$.

For a triply degenerate mode ($T_d$ symmetry), in the frame of this approximation, the components of $p$ are given by

$$\begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix} = -a \begin{pmatrix} Q_x \\ Q_y \\ Q_z \end{pmatrix}.$$

Therefore, $a$ is simply given by

$$a = -\partial p_x/\partial Q_x = -\partial p_y/\partial Q_y = -\partial p_z/\partial Q_z.$$

In the case of $C_{3v}$ symmetry ($z$ being along the trigonal axis), the components of $p$ are given by

$$\begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix} = -a_l \begin{pmatrix} 0 \\ 0 \\ Q_z \end{pmatrix} \qquad \begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix} = -a_t \begin{pmatrix} Q_x \\ Q_y \\ 0 \end{pmatrix}$$

for a longitudinal mode and for a transverse one, respectively. Therefore

$$a_l = -\partial p_z/\partial Q_z \qquad a_t = -\partial p_x/\partial Q_x = -\partial p_y/\partial Q_y.$$

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