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2007 J. Phys.: Condens. Matter 19 456219

(http://iopscience.iop.org/0953-8984/19/45/456219)

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **19** (2007) 456219 (5pp) doi:10.1088/0953-8984/19/45/456219

Determination of 'bisotropic' stresses in layered semiconductor structures from Raman light scattering data

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Received 6 March 2007, in final form 10 September 2007
Published 17 October 2007
Online at stacks.iop.org/JPhysCM/19/456219

Abstract

Explicit expressions are derived for phonon frequency shifts observed in Raman experiments under conditions of isotropic biaxial ('bisotropic') stress in the plane of a (111)-oriented cubic crystal. Like in the well-studied case of (001)-oriented crystal, a phonon doublet and a phonon singlet are formed. But as distinct from the (001) crystal orientation case, where the singlet outstrips the doublet with increase in stress, in the case of (111) orientation, in contrast, the doublet outstrips the singlet. In the latter case the effect as a whole is quantitatively smaller. In addition, in both cases, exclusively simple formulae are obtained which allow the expression of Raman shifts under bisotropic stress in terms of shifts under uniaxial deformations of the same material. In this approach one does not need to know in advance both phonon deformation potentials and elastic constants of the material.

1. Introduction

Semiconductor device structures as a rule consist of a number of layers made of different materials. Therefore the presence in them of internal stresses takes on great importance because they can change the electrical properties of the individual layers. Recently, Raman light scattering spectroscopy has been used actively for measuring such stresses. But formulae available for conversion of observed shifts of phonon frequency into stresses assume only one specific orientation for crystals of cubic symmetry; namely (001) orientation, which is the one most frequently encountered in practice (see, for example, review [1] and the papers cited there).

However, (111)-oriented crystalline layers can also occur [2]. Therefore it is a good idea to have similar explicit expressions for them. It should be noted also that so-called phonon deformation potentials entering such the formulae are determined from experiment and are revised from time to time: for example in [3–5] for Si, in [6] for ZnS; therefore they

cannot be considered as reliably established. Microscopic calculations of the above mentioned phenomenological parameters in the frameworks of both classical [5, 7–9] and quantum [10] mechanics reduce them to other (force) constants in the expression for the total energy of the crystal, which in turn have to be determined from experiment.

This paper has a twofold purpose. In the first place we derive the formulae that connect the phonon frequency shifts observed in Raman experiments with the bisotropic stress in the plane of the surface for (111)-oriented cubic crystal. The second goal is to show the possibility of simple calculation of a Raman shift–bisotropic stress relation from the Raman spectroscopy data for the same material subjected to uniaxial deformations. In this approach one does not need to know in advance both the phonon deformation potentials and elastic constants of the material.

2. Calculation of phonon frequency shifts in (111)-oriented cubic crystal under bisotropic stress

From the dynamical equations for a crystal lattice of diamond type one obtains the following secular equation for the frequency ω of the triply degenerate (at the wavevector $k = 0$) optical phonon in the presence of strain [1, 3, 8]:

$$\begin{vmatrix} pu_{xx} + q(u_{yy} + u_{zz}) - \lambda & 2ru_{xy} & 2ru_{xz} \\ 2ru_{xy} & pu_{yy} + q(u_{zz} + u_{xx}) - \lambda & 2ru_{yz} \\ 2ru_{xz} & 2ru_{yz} & pu_{zz} + q(u_{xx} + u_{yy}) - \lambda \end{vmatrix} = 0, \quad (1)$$

where p, q and r are phenomenological parameters (phonon deformation potentials), $\lambda = \omega^2 - \omega_0^2 \approx 2\omega_0(\omega - \omega_0) \equiv 2\omega_0\Delta\omega$, ω_0 is the undisturbed (degenerate) phonon frequency, u_{ij} is the strain tensor given in the system of crystallographic axes [100], [010] and [001]. In the above equation, deformation is considered as small (i.e. elastic). In the elasticity region the strain tensor components u_{ij} are related to components of the stress tensor σ_{ij} by Hooke's law

$$u_{ij} = \sum_{kl} S_{ijkl}\sigma_{kl}, \quad (2)$$

where the S_{ijkl} are the components of elastic compliance tensor (in crystals of cubic symmetry only three independent components are available: $S_{xxxx} \equiv S_{11}$, $S_{xxyy} \equiv S_{12}$ and $S_{yzyz} \equiv S_{44}$).

For biaxial stress in the plane of the surface of (001)-oriented crystal the stress tensor takes an especially simple form [11]:

$$\hat{\sigma}_{(001)} = \begin{pmatrix} \sigma_{xx} & 0 & 0 \\ 0 & \sigma_{yy} & 0 \\ 0 & 0 & 0 \end{pmatrix}; \quad (3)$$

hence from (1), the known expressions for the doublet and the singlet follow immediately:

$$\Delta\omega_{1,2}^{(001)}|_{bi} = \frac{\sigma}{2\omega_0}\left[p(S_{11} + S_{12}) + q(S_{11} + 3S_{12})\right], \quad (4d)$$

$$\Delta\omega_{3}^{(001)}|_{bi} = \frac{\sigma}{\omega_0}\left[pS_{12} + q(S_{11} + S_{12})\right], \quad (4s)$$

where it is assumed that biaxial stress is isotropic in the plane of the interface as is the case mostly in practice, i.e. $\sigma_{xx} = \sigma_{yy} = \sigma$ (a 'bisotropic' stress in accordance with the definition in [12]). Thus threefold degeneracy of the phonon frequency is lifted only partially.

The eigenvector corresponding to the singlet solution (4*s*) is directed along the [001] axis determining the polarization direction of lattice vibration in this mode. And the eigenvectors of the doublet solution (4*d*) characterize the remaining two vibration modes polarized in the

plane perpendicular to this axis. It should be noted that this picture coincides with the situation where uniaxial stress is applied along the [001] axis [3, 8].

If the crystal is a (111)-oriented one, the stress tensor (in the crystallographic coordinate system) appears as

$$\hat{\sigma}_{(111)} = \sigma \begin{pmatrix} (1+\cos^2\theta)/2 & (\cos^2\theta - 1)/2 & -\sin\theta\cos\theta/\sqrt{2} \\ (\cos^2\theta - 1)/2 & (1+\cos^2\theta)/2 & -\sin\theta\cos\theta/\sqrt{2} \\ -\sin\theta\cos\theta/\sqrt{2} & -\sin\theta\cos\theta/\sqrt{2} & \sin^2\theta \end{pmatrix}, \quad (5)$$

where $\theta = \arcsin(\sqrt{2/3}) = \arccos(\sqrt{1/3})$. In this case, from (1) the doublet and singlet are obtained as well, but they are completely different:

$$\Delta\omega_{1,2}^{(111)}|_{bi} = \frac{\sigma}{3\omega_0}\left[(p+2q)(S_{11}+2S_{12}) + rS_{44}/2\right], \quad (6d)$$

$$\Delta\omega_{3}^{(111)}|_{bi} = \frac{\sigma}{3\omega_0}\left[(p+2q)(S_{11}+2S_{12}) - rS_{44}\right]. \quad (6s)$$

In particular, as distinct from the (001) orientation case for the crystal, in the case of its (111) orientation the phonon frequency shifts depend on all three deformation potentials p, q and r. In this case the singlet vibration mode proves to be polarized along the [111] axis and the remaining two modes are polarized in the plane perpendicular to this direction. We have here an analogy with the case of uniaxial stress along the [111] axis [3, 8].

Along with p, q and r, (6) (like (4)) does require reliable knowledge of all three elastic constants of the material. However we will show below that it is possible to manage without all this when having at one's disposal the results of Raman measurements for the same material under conditions of uniaxial deformations.

3. Calculation of phonon frequency shifts under bisotropic stress in terms of the shifts under uniaxial stresses

Using the explicit expressions for phonon frequency shifts under conditions of uniaxial deformations (see, for example, [3, 4, 8]) and introducing the slopes $k_i^{[j]}$ ($i = s, d$, $j =$ [001], [111]) for linear dependences of the doublet and the singlet on the stress along the [001] axis:

$$\Delta\omega_d^{[001]} = k_d^{[001]}\sigma, \qquad k_d^{[001]} = [pS_{12} + q(S_{11}+S_{12})]/2\omega_0 \quad (7d)$$

$$\Delta\omega_s^{[001]} = k_s^{[001]}\sigma, \qquad k_s^{[001]} = (pS_{11} + 2qS_{12})/2\omega_0 \quad (7s)$$

and, for example, for the doublet under stress along the [111] axis:

$$\Delta\omega_d^{[111]} = k_d^{[111]}\sigma, \qquad k_d^{[111]} = [(p+2q)(S_{11}+2S_{12}) - rS_{44}]/6\omega_0 \quad (8)$$

one can determine the material parameters p, q and r in terms of the slopes $k_i^{[j]}$:

$$\begin{aligned} p &= \frac{2\omega_0[S_{12}(2k_d^{[001]}/k_s^{[001]} - 1) - S_{11}]k_d^{[001]}}{(2S_{12}^2 - S_{11}^2 - S_{11}S_{12})k_d^{[001]}/k_s^{[001]}}, \\ q &= \frac{2\omega_0(S_{12} - S_{11}k_d^{[001]}/k_s^{[001]})k_d^{[001]}}{(2S_{12}^2 - S_{11}^2 - S_{11}S_{12})k_d^{[001]}/k_s^{[001]}}, \\ r &= \frac{(p+2q)(S_{11}+2S_{12}) - 6\omega_0 k_d^{[111]}}{S_{44}}. \end{aligned} \quad (9)$$

Table 1. Experimental (for [001] and [111] stresses) and calculated (using formulae (10)–(11), for bisotropic stress) slopes for stress dependences of the phonon frequency shifts in silicon.

	$T = 300$ K		$T = 110$ K
Type of deformation	k_s and k_d [3] (cm^{-1} GPa^{-1})	k_s and k_d [4] (cm^{-1} GPa^{-1})	k_s and k_d [5] (cm^{-1} GPa^{-1})
Along [001] axis	$k_s = 0.5$ $k_d = 1.91$	$k_s = 0.8$ $k_d = 2.0$	$k_s = 1.07$ $k_d = 2.27$
Along [111] axis	$k_s = 3.32$ $k_d = 1.15$	$k_s = 2.8$ $k_d = 0.9$	$k_s = 3.5$ $k_d = 1.13$
Bisotropic, (001) wafer	$k_s = 3.82$ $k_d = 2.41$	$k_s = 4.0$ $k_d = 2.8$	$k_s = 5.54$ $k_d = 3.34$
Bisotropic, (111) wafer	$k_s = 2.30$ $k_d = 3.17$	$k_s = 1.8$ $k_d = 3.90$	$k_s = 2.26$ $k_d = 4.48$

Substituting these expressions into (4) we obtain very simple formulae for frequency shifts under bisotropic stress in (001)-oriented crystal:

$$\Delta\omega_d^{(001)}|_{bi} = (k_s^{[001]} + k_d^{[001]})\sigma, \tag{10d}$$

$$\Delta\omega_s^{(001)}|_{bi} = 2k_d^{[001]}\sigma, \tag{10s}$$

and substitution of (9) into (6) gives rise to similar formulae for (111)-oriented crystal:

$$\Delta\omega_d^{(111)}|_{bi} = (k_s^{[001]} + 2k_d^{[001]} - k_d^{[111]})\sigma, \tag{11d}$$

$$\Delta\omega_s^{(111)}|_{bi} = 2k_d^{[111]}\sigma. \tag{11s}$$

Thus knowledge of the slopes for stress dependences of phonon shifts under uniaxial deformations allows calculation of the relations between phonon shifts and the bisotropic stress (without knowledge of any material parameters).

4. Examples and conclusion

Let us use for illustration the uniaxial stress dependences of the doublet and singlet in silicon from the papers [3–5] (the slopes are taken directly from the graphics, i.e. with some error). The experimental and calculated results are brought together in table 1.

Unfortunately, papers where the slopes for stress dependences of phonon shifts under bisotropic deformations have been measured experimentally are not known to the author. Furthermore, measuring such dependences is very difficult because of the impossibility of controlling the bisotropic stress smoothly. But one can compare the results from the given approach with the results of detailed calculations from [11] (through particular parameters) for bisotropic stress in (001)-oriented silicon crystal: a relation $\sigma = 2.49 \times 10^9$ dyn $\mathrm{cm}^{-2} \cdot \Delta\omega$ (cm^{-1}) was obtained in that paper for the singlet. The inverse relation is $\Delta\omega(\mathrm{cm}^{-1}) = 4 \cdot \sigma$ (GPa), in full agreement with our approach (on the basis of data from [4]). Earlier data from [3] give this result approximately.

It is follows from table 1 that for all cases studied, for (001)-oriented silicon crystal the singlet outstrips the doublet with increase in the stress but for (111)-oriented crystal, in contrast, the doublet outstrips the singlet. In the latter case the frequency shift, as a whole, is somewhat smaller. Therefore (001)-oriented silicon crystal is preferable to (111)-oriented material from the point of view of sensitivity to Raman measurements.

It is evident that electrical properties of (001)-oriented silicon wafers may also be influenced by the bisotropic stress in a more significant way than those of (111)-oriented wafers. Therefore when there is a question of undesired deformation of the silicon crystal, for example, for the coating layer, (111)-oriented material is preferable. In contrast, if the biaxial deformation is used intentionally—for changing electrical properties of the underlying silicon crystal—then the (001) orientation should be preferred.

Acknowledgment

The author is grateful to the Laboratory of Physical Sensors (Institute of Semiconductor Physics, Kiev) headed by Dr Yu M Shwarts for financial support.

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