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## Utilization of the sum rule for construction of advanced dispersion model of crystalline silicon containing interstitial oxygen

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### ABSTRACT

The distribution of the total transition strength, i.e. the right hand side of the integral form of Thomas–Reiche–Kuhn sum rule, into individual absorption processes is described for crystalline silicon containing interstitial oxygen. Utilization of the sum rule allows the construction of a dispersion model covering all elementary excitations from phonon absorption to core electron excitations. The dependence of transition strength of individual electronic and phonon contributions on temperature and oxygen content is described.

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### 1. Introduction

The classical theory of dispersion provides three general conditions for the linear dielectric response that physically consistent models must satisfy [1–4]: Kramers–Kronig relation, time reversal symmetry and sum rule. While the first two conditions are well known and widely used in construction of dispersion models, the sum rule is rarely utilized. Classical  $f$ -sum rule is usually expressed for the imaginary part of dielectric function  $\varepsilon_i$  as follows

$$\int_0^{\infty} \varepsilon_i(\omega) \omega \, d\omega = \frac{\pi}{2} \omega_p^2, \quad (1)$$

where  $\omega$  is light frequency and  $\omega_p$  is a constant called the plasma frequency. In the frame of classical physics plasma frequency is proportional to density of electrons  $\mathcal{N}_e$

$$\omega_p^2 = \frac{e^2 \mathcal{N}_e}{\epsilon_0 m_e}, \quad (2)$$

where  $e$ ,  $\epsilon_0$  and  $m_e$  are physical constants, i.e. electron charge, vacuum permittivity and electron mass. It is clear that Eq. (1) together with Eq. (2) form a bridge between dielectric response and structural parameters of the system such as atomic or mass density. One reason why the sum rule is seldom used for construction of dispersion models is that it is a global condition which can be applied correctly only to the entire

dielectric response covering all elementary excitations of the system. However, thanks to the progress in instrumentation we are nowadays able to measure dielectric response in broad spectral range from far infrared (FIR) to vacuum ultraviolet (VUV) using commercial table top instruments. Moreover, using synchrotron facilities it is possible to extend the spectral range to the X-ray region and cover the full range of electronic excitations in solids. Therefore, modeling of the complete dielectric response in the entire spectral region has become important.

Silicon wafers are widely used as substrates both in the microelectronic industry and fundamental research of thin films. Although the ideal substrates would be pure silicon single crystals, in practice silicon wafers produced using Czochralski process [5] are mostly utilized. In general, these wafers differ from ideal Si crystals by the presence of interstitial oxygen ( $O_i$ ) and concentration of dopants [6]. Moreover, the concentrations of interstitial oxygen and dopants differ between wafers and even within one wafer. Therefore, it is not possible to use single tabulated optical constants for all Si pieces, especially in the IR region, and models describing the dielectric function of real silicon wafers must be developed. It is also important that such models should contain the minimum numbers of parameters necessary to express the variations between individual silicon wafers. This means that models should be parametrized by concentration of interstitial oxygen, oxygen precipitates [7], substitutional carbon [8] and dopants such as boron, phosphorus or arsenic. In addition, since the optical measurements can be carried out at different temperatures, the models should also include temperature as a parameter.

In this work it will be shown how the sum rule can be utilized for construction of dispersion model of c-Si wafers applicable in the entire spectral region from FIR to VUV. This model will be temperature dependent, nevertheless, it will only contain the influence of interstitial oxygen which is perhaps the most important effect since interstitial

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oxygen is present in all Czochralski wafers [9]. The presented results summarize ellipsometric and spectrophotometric characterizations of a set of double side polished wafers and slabs produced using float zone and Czochralski processes. Data sets from several instruments were combined to cover a wide spectral range from 8.7 meV (70 cm<sup>-1</sup>) to 8.7 eV and temperature range from 300 to 600 K. Experimental details are out of scope of this paper and will be published elsewhere.

**2. Theoretical background**

Thomas–Reiche–Kuhn (TRK) sum rule for system of N<sub>e</sub> electrons can be written as [10]

$$\sum_{f \neq i} \frac{2}{m_e} \frac{|\langle f | \hat{p}_{xe} | i \rangle|^2}{E_f - E_i} = \sum_{f \neq i} f_{if} = N_e, \tag{3}$$

where m<sub>e</sub> and  $\hat{p}_{xe}$  denote electron mass and total momentum operator of electrons, respectively. The symbols |i⟩ and |f⟩ represent a complete set of many-body eigenstates of the system with eigenvalues of energy E<sub>i</sub> and E<sub>f</sub>. The quantity f<sub>if</sub> is called oscillator strength. It was shown that the discrete TRK sum rule (3) can be rewritten in an integral form [11]

$$\int_0^\infty \mathcal{F}_e(E) dE = \frac{N_e}{V} = \mathcal{N}_e, \tag{4}$$

where V is volume of the system and the transition strength function  $\mathcal{F}_e$  is defined as

$$\mathcal{F}_e(E) = \frac{1}{V} \sum_{f \neq i} f_{if} [\delta(E_f - E_i - E) + \delta(E_i - E_f - E)]. \tag{5}$$

The same TRK sum rule can be also written for nuclei

$$\int_0^\infty \mathcal{F}_n(E) dE = \mathcal{N}_n, \tag{6}$$

where n distinguishes the type of nuclei (n = Si or O for silicon containing interstitial oxygen) and  $\mathcal{N}_n$  are the corresponding nuclei densities.

Within dipole approximation the three quantum-mechanical transition strength functions  $\mathcal{F}_e$ ,  $\mathcal{F}_{Si}$  and  $\mathcal{F}_O$  can be linearly combined to form a new quantity F, also called (optical) transition strength function, directly related to the dielectric function:

$$F(E) = \mathcal{M}^{-1} \left[ \mathcal{F}_e(E) + \sum_n \frac{Z_n^2 m_e}{m_n} \mathcal{F}_n(E) \right] \approx \varepsilon_i(E) E, \tag{7}$$

where  $\mathcal{M}^{-1} = (eh)^2 / (8\pi\epsilon_0 m_e)$  is a combination of fundamental physical constants and the symbols Z<sub>n</sub> and m<sub>n</sub> denote the proton number and mass of nucleus n, respectively. The transition strength function F satisfies the following sum rule which is a linear combination of the TRK sum rules (4) and (6):

$$\int_0^\infty F(E) dE = \mathcal{M}^{-1} \left( \mathcal{N}_e + \sum_n \frac{Z_n^2 m_e}{m_n} \mathcal{N}_n \right) = N. \tag{8}$$

The quantity N on the right hand side is called total transition strength of the system. Thus, the transition strength function is the spectral distribution of the transition strength. Utilization of the sum rule for construction of dispersion models consists in the distribution of total transition strength among individual contributions of elementary excitations [11–13].

The symbol ≈ in formula (7) is used to emphasize that the quantum mechanical quantity F(E) and macroscopic quantity ε<sub>i</sub> representing dielectric response are connected by the dipole approximation. Within

classical physics this distinction disappears and the description using transition strength function is equivalent to other representations of linear dielectric response:

$$F(E) = E \varepsilon_i(E) = \frac{\hbar}{\epsilon_0} \sigma_r(E), \tag{9}$$

where σ<sub>r</sub> is the real part of conductivity. The linear dielectric response is then given as the sum of damped harmonic oscillators (DHOs):

$$F(E) = \frac{4}{\pi} \sum_j \frac{N_j B_j E^2}{(E_{c,j}^2 - E^2)^2 + 4B_j^2 E^2}, \quad \sum_j N_j = N, \tag{10}$$

where N<sub>j</sub>, E<sub>c,j</sub> and B<sub>j</sub> are the transition strength, central energy and broadening of DHO, respectively. The quantity N<sub>j</sub> has unit eV<sup>2</sup> and is also often called oscillator strength even though it differs from unitless quantity f<sub>if</sub> occurring in Eq. (3). In formula (10) the terms satisfying inequality E<sub>c,j</sub> > B<sub>j</sub> can be rewritten by the Lorentz functions:

$$F_j(E) = \frac{N_j B_j E}{\pi E_j} \left( \frac{1}{(E_j - E)^2 + B_j^2} - \frac{1}{(E_j + E)^2 + B_j^2} \right), \tag{11}$$

where E<sub>j</sub> is the energy of transition related to the central energy of DHO by relation E<sub>c,j</sub><sup>2</sup> = E<sub>j</sub><sup>2</sup> + B<sub>j</sub><sup>2</sup>.

Note that classical systems with parameters E<sub>c,j</sub> < B<sub>j</sub> (overdamped oscillators) or E<sub>c,j</sub> = 0 (Drude formula) are impossible to describe using Eq. (11) as Lorentzian broadened discrete spectrum. Formula (11) is equivalent to quantum mechanical description represented by Eq. (5) for limit B<sub>j</sub> → 0. On the other hand, quantum mechanical systems exhibit behavior that cannot be described using a finite number of DHOs, for instance bandgap. Moreover, Gaussian broadening is usually more appropriate for quantum systems [14].

The approach based on the transition strength function takes advantage of a clear connection between dielectric response and microscopic quantities as oscillator strengths or momentum matrix elements. If N<sub>j</sub> is the transition strength of an individual transition i → j corresponding to absorbed energy E<sub>j</sub> = E<sub>f</sub> - E<sub>i</sub> then it holds:

$$N_j = \frac{\mathcal{M}^{-1}}{V} f_{if} = \frac{(eh)^2}{8\pi\epsilon_0 m_e V} f_{if} = \frac{(eh)^2}{4\pi\epsilon_0 m_e^2 V E_j} |\langle f | \hat{p}_{xe} | i \rangle|^2. \tag{12}$$

The constant  $\mathcal{M}$  represents a link between optical quantities, i.e. transition strength, and density of the system. For example, if N<sub>ex</sub> is the transition strength of an excitonic peak then the relation

$$N_{ex} = \frac{\mathcal{M}^{-1}}{V} \sum_f f_{if} = \mathcal{M}^{-1} \mathcal{N}_{ex} \tag{13}$$

gives the ‘volume density of excitons’  $\mathcal{N}_{ex}$  (the summation is performed over f states representing all the excitonic excitations). However, it is not clear how is such quantity related to the density of real particles (electrons, nuclei). Since all elementary excitations in solids involve quasiparticles the only formula with a clear interpretation is Eq. (8) for total transition strength N. For a more detailed discussion see [11].

**3. Absorption processes in c-Si wafers**

The absorption in c-Si wafers is caused by the following effects corresponding to the individual contributions to the transition strength function:

- dt Direct interband transitions from valence to conduction band.
- idt Indirect interband transitions from valence to conduction band.

- fc Indirect intraband transitions in valence and conduction bands, i.e. contribution of free carriers.
- vx Excitations of valence electrons to higher energy states above the conduction band.
- K, L Excitations of electrons from the core levels to the electron states above the Fermi energy.
- 1 ph One-phonon absorption, i.e. excitation of vibrational states of Si nuclei. It is forbidden by selection rules for ideal c-Si, however, it is present in real wafers due to the presence of imperfections and foreign atoms.
- mph Multi-phonon absorption, in our model considered up to four phonons, i.e.  $mph = 2 \text{ ph} + 3 \text{ ph} + 4 \text{ ph}$ .
- $A_{2u}$  One-phonon absorption corresponding to antisymmetric stretching vibrational mode of interstitial oxygen nuclei.
- $A_{2u} + A_{1g}$  Two-phonon absorption corresponding to combination of  $A_{2u}$  and  $A_{1g}$  vibrational modes of interstitial oxygen nuclei.

General ideas that can be used for construction of dispersion models related to individual absorption processes are given in [11]. Application of these ideas to amorphous hydrogenated silicon (a-Si:H) is shown in [12,13]. Detailed description of individual dispersion models for c-Si is out of this paper because it deals with dependences of integral transition strength of individual processes on temperature and concentration of interstitial oxygen.

#### 4. Distribution of the transition strength

The total transition strength  $N$  is the sum of contributions of electrons and nuclei of Si and O, i.e.

$$N = N_e + N_{Si} + N_O. \quad (14)$$

All the individual contributions depend on temperature  $T$  and atomic fraction of interstitial oxygen  $f_{O_i}$ , as follows

$$N_e(T, f_{O_i}) = [Z_{Si}(1-f_{O_i}) + Z_O f_{O_i}] N_a(T), \quad (15)$$

$$N_{Si}(T, f_{O_i}) = \frac{Z_{Si}^2 m_e}{m_{Si}} (1-f_{O_i}) N_a(T), \quad (16)$$

$$N_O(T, f_{O_i}) = \frac{Z_{Si}^2 m_e}{m_O} f_{O_i} N_a(T). \quad (17)$$

Symbols  $Z_{Si}$ ,  $Z_O$ ,  $m_{Si}$  and  $m_O$  denote proton number of Si, proton number of O, mass of Si nucleus and mass of O nucleus, respectively. The density parameter  $N_a$  depends on temperature as follows

$$N_a(T) = N_a(300 \text{ K}) \left[ \frac{1 + e(300 \text{ K})}{1 + e(T)} \right]^3 \quad (18)$$

where  $e(T)$  is the linear thermal expansion coefficient [15] and  $N_a(300 \text{ K}) = 108.2 \text{ eV}^2$  [11]. The thermal dependence of  $N_a$  is illustrated in Fig. 1 for the temperature range 300–1000 K. In principle,  $N_a$  depends also on the concentrations of impurities, but this dependence can be disregarded [8] for common concentrations.

From the point of view of absorption processes the total transition strength  $N$  can be split into electron excitation  $N_{ee}$  and phonon  $N_{ph}$  parts:

$$N = N_{ee} + N_{ph}. \quad (19)$$

Even though the electron excitation transition strength  $N_{ee}$  differs from the electronic part  $N_e$  of the sum introduced in Eq. (14) their values are very close. This is because  $N = N_e \mathcal{U}$ , where  $\mathcal{U}$  is close to unity,

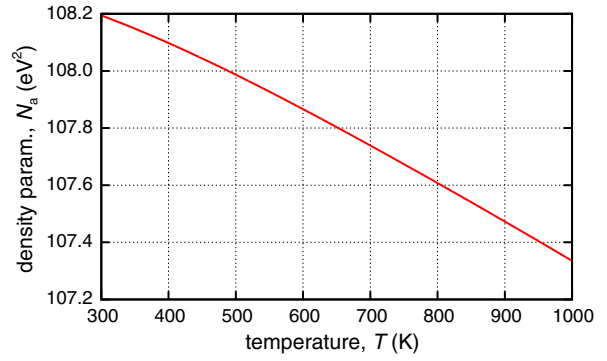


Fig. 1. Temperature dependence of density parameter  $N_a$  for c-Si calculated using Eq. (18).

specifically for silicon  $\mathcal{U} = 1.0002735$ , while for  $N_{ph}$  it holds  $N_{ph} < N_{Si} + N_O$  [11]. Hence both differ from  $N$  only slightly and thus

$$N \approx N_{ee} \approx N_e \approx Z_{Si} N_a, \quad (20)$$

where  $Z_{Si} = 14$  is the approximate mean number of electrons per atom in silicon wafers. It is evident that temperature dependence of  $N_{ee}$  is then given by the temperature dependence of  $N_a$  in Eq. (18).

#### 4.1. Transitions above the bandgap

The dielectric response above the bandgap, i.e. K, L, vx and vc (interband valence-to-conduction transitions  $vc = dt + idt$ ) absorption processes, is insensitive to presence of interstitial oxygen in concentrations typical for Czochralski silicon. Therefore, the dependence of all electronic transitions on parameter  $f_{O_i}$  can be disregarded.

Concerning temperature, the transition strengths  $N_t$  of individual contributions  $t = K, L, vx, vc$  depend on temperature only through  $N_a$ . The spectral distribution of transition strength of electronic excitations is of course temperature dependent as shown in Fig. 2 for 300 and 600 K. Therefore, it is useful to introduce the effective number of electrons  $n_t$  via the following relation:

$$N_t(T) = n_t N_a(T). \quad (21)$$

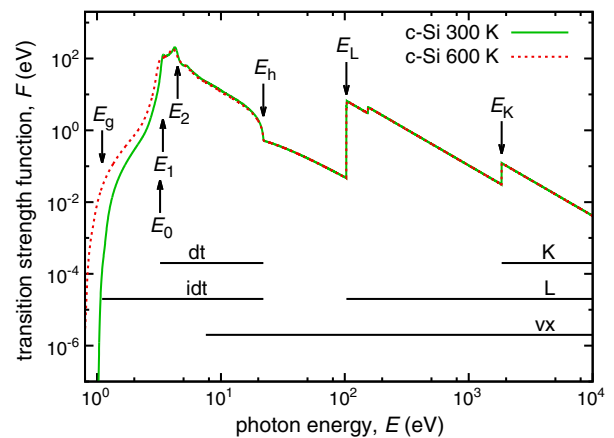


Fig. 2. Spectral distribution of transition strength of c-Si in the region of electronic excitations above the bandgap for two selected temperatures. Important energies are marked with arrows:  $E_g$  – minimum energy of interband transitions (bandgap);  $E_1$  – energy of 1st direct transition structure;  $E_2$  – energy of 2nd direct transition structure;  $E_h$  – maximum energy of interband transitions;  $E_L$  – minimum energy of core level L-electron excitations; and  $E_K$  – minimum energy of core level K-electron excitations.

The effective number of electrons  $n_t$  defined in this way is then temperature independent. It is also possible to introduce the effective number of valence electrons  $n_{ve}$  as

$$n_{ve} = n_{vc} + n_{vx}. \quad (22)$$

The effective numbers  $n_{ve}$ ,  $n_L$  and  $n_K$  are not equal to the numbers of electrons in the corresponding shells, i.e. 4, 8 and 2, respectively. However, their sum must correspond to the number of electrons in Si:

$$n_{ve} + n_L + n_K \approx Z_{Si} = 14. \quad (23)$$

It was shown that values  $n_{ve} = 4.12$ ,  $n_L = 8.33$  and  $n_K = 1.55$  calculated by Shiles for aluminum [16] can be used for a-Si:H if the measurements do not extend to the X-ray region [12,13]. These values should be suitable also for crystalline silicon.

It follows from the foregoing that the effective number of electrons calculated up to a certain energy  $E$

$$n_{eff}(E) = \frac{1}{N_a(T)} \int_0^E F(E') dE' \quad (24)$$

is a useful quantity since it can be interpreted as the sum per one atom. Its limit for  $E \rightarrow \infty$  is

$$n_{eff}(\infty) = [Z_{Si}(1-f_{O_i}) + Z_{O_i}f_{O_i}]u \approx 14. \quad (25)$$

The course of  $n_{eff}(E)$  is plotted in Fig. 3 for the same two temperatures as in Fig. 2. It is practically identical for both the temperatures except for the region of interband transitions which is shown in the inset. It is interesting that  $n_{eff}(E)$  starts to increase significantly above the onset of direct transitions  $E_0$ , and not from the band gap  $E_g$ .

Similar to Eq. (21) we can introduce the effective numbers of electrons also for  $t = dt$ ,  $idt$

$$N_t(T) = n_t(T)N_a(T), \quad (26)$$

but they depend on temperature. The dependence of  $n_{idt}(T)$  on temperature is almost linear and it is given by the following formula [17,18,11]:

$$n_{idt}(T) \propto 1 + 2f^{BE}(E_p, T) = 1 + \frac{2}{\exp(E_p/k_B T) - 1}, \quad (27)$$

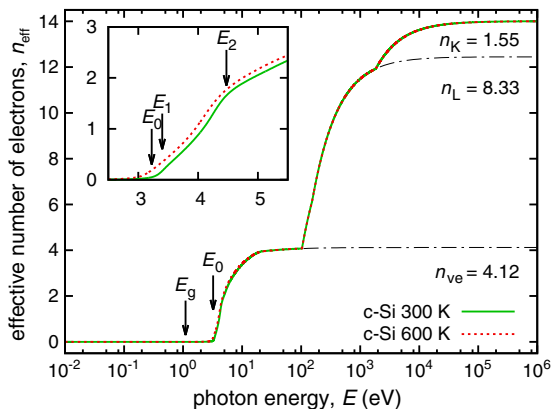


Fig. 3. The evolution of effective number of electrons  $n_{eff}$  with photon energy calculated using Eq. (24) for two selected temperatures. Dash-and-dot lines extrapolate ve and L contributions above  $E_L$  and  $E_K$  energies. The inset shows the region of onset of direct interband electronic transitions in detail.

Table 1 Effective numbers of electrons corresponding to the individual absorption processes for selected temperatures. Note that  $n_{ve} = n_{vx} + n_{vc}$ ,  $n_{vc} = n_{idt} + n_{dt}$  and  $n_{mph} = n_{2ph} + n_{3ph} + n_{4ph}$ . The last column describes the approximate temperature dependence.

	300 K	400 K	500 K	600 K	
<i>Above <math>E_g</math></i>					
$n_K$	1.55				Const.
$n_L$	8.33				Const.
$n_{ve}$	4.12				Const.
$n_{vx}$	0.24				Const.
$n_{vc}$	3.88				Const.
$n_{idt}$	0.50	0.61	0.72	0.84	Lin.
$n_{dt}$	3.38	3.27	3.16	3.04	Lin.
<i>below <math>E_g</math></i>					
$n_{fc}$	$3.23 \times 10^{-12}$	$1.01 \times 10^{-9}$	$3.42 \times 10^{-8}$	$3.76 \times 10^{-7}$	Exp.
$n_{mph}$	$1.16 \times 10^{-7}$	$1.48 \times 10^{-7}$	$1.84 \times 10^{-7}$	$2.22 \times 10^{-7}$	Lin.
$n_{2ph}$	$1.00 \times 10^{-7}$	$1.26 \times 10^{-7}$	$1.52 \times 10^{-7}$	$1.79 \times 10^{-7}$	Lin.
$n_{3ph}$	$1.51 \times 10^{-8}$	$2.08 \times 10^{-8}$	$2.84 \times 10^{-8}$	$3.78 \times 10^{-8}$	Quad.
$n_{4ph}$	$1.09 \times 10^{-9}$	$1.91 \times 10^{-9}$	$3.17 \times 10^{-9}$	$5.01 \times 10^{-9}$	Cubic

where  $f^{BE}$  denotes Bose-Einstein statistics,  $k_B$  is the Boltzmann constant and  $E_p$  is the effective mean energy of phonons participating in the indirect interband transitions. The dependence of  $n_{dt}(T)$  follows from

$$n_{idt}(T) + n_{dt}(T) = n_{vc}. \quad (28)$$

The values of effective numbers of electrons are tabulated for selected temperatures in Table 1.

#### 4.2. Transitions below the bandgap

Transitions below the bandgap include phonon and free carriers absorption processes. The transition strength in spectral region where these processes are important is plotted for selected temperatures from 300 to 600 K in Fig. 4. Note that the curves correspond to pure c-Si hence no one-phonon absorption is present. The phonon contribution to the sum is then dominated by two-phonon absorption processes. Therefore, temperature dependence of  $N_{mph}$  is practically linear around and above room temperature because phonon occupation numbers depend on temperature linearly in the considered range. This linear dependence can be seen in Fig. 5 showing  $N_{mph}$  of pure c-Si calculated from the temperature dependence of all multi-phonon processes [19,

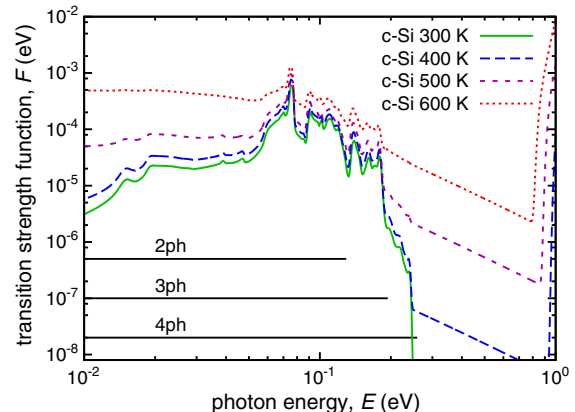


Fig. 4. Spectral distribution of transition strength of pure c-Si in the region of phonon and free carrier absorption below the bandgap for selected temperatures.

11]. The transition strength of free carriers is also plotted in this figure. The free carrier part is given by the well-known expression [20]:

$$N_{fc} \propto T^3 \exp\left(-\frac{E_g}{2k_B T}\right). \quad (29)$$

The values of effective numbers of electrons corresponding to free carriers and phonons are tabulated for selected temperatures in Table 1. In this table multi-phonon absorption is split to individual contributions 2 ph, 3 ph and 4 ph. It can be seen that transition strengths of 3 ph and 4 ph contributions are 10 and 100 times smaller than 2 ph. It is clear that contribution of free carriers and phonons to the sum is insignificant even though it is certainly not negligible from the point of view of dielectric response.

In contrast to electronic excitations, the dielectric response corresponding to phonon absorption processes depends considerably on concentration of interstitial oxygen. In Fig. 6 the transition strength functions at room temperature is plotted for pure c-Si and typical Czochralski silicon with 20 ppm of interstitial oxygen (c-Si: O<sub>20</sub>). The contribution to transition strength function caused by interstitial oxygen is proportional to its atomic fraction  $f_{O_i}$ .

The most prominent structure corresponds to antisymmetric stretching vibrational mode of O<sub>i</sub> at 1107 cm<sup>-1</sup> labeled as A<sub>2u</sub>. The transition strength of this vibrational mode was assumed as follows:

$$N_{A_{2u}} = \alpha_{A_{2u}} N_{O_i}, \quad (30)$$

where  $N_{O_i}$  is given by formula (17) and the relative transition strength  $\alpha_{A_{2u}} = 0.1914$  corresponds to the effective charge of 3.5e determined by ab initio calculations [21]. Note that the value of  $\alpha_{A_{2u}}$  calculated from the relation between O<sub>i</sub> concentration and  $\alpha$  determined by another independent method such as ASTM F1188 [22]. The obtained value of  $\alpha_{A_{2u}}$  was approximately 5% larger than the value given above.

Other O<sub>i</sub> vibrational modes are not IR active. However, a two-phonon A<sub>2u</sub> + A<sub>1g</sub> absorption peak can be observed at 1721 cm<sup>-1</sup> [23]. In contrast to one-phonon A<sub>2u</sub> vibrational mode, the strength of this two-phonon vibrational mode is temperature dependent:

$$N_{A_{2u}+A_{1g}} = \alpha_{A_{2u}+A_{1g}}(T) N_{O_i}, \quad (31)$$

where relative transition strength is given as follows:

$$\alpha_{A_{2u}+A_{1g}}(T) = \alpha_{A_{2u}+A_{1g}}(300\text{ K}) \frac{f_{A_{2u}+A_{1g}}(T)}{f_{A_{2u}+A_{1g}}(300\text{ K})}, \quad (32)$$

$$f_{A_{2u}+A_{1g}}(T) = f^{BE}(E_{A_{2u}}, T) + f^{BE}(E_{A_{1g}}, T) + 1. \quad (33)$$

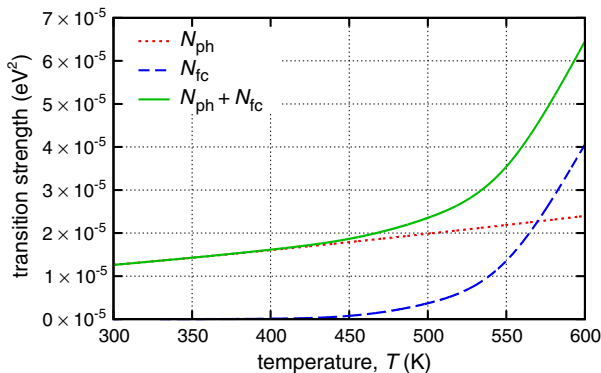


Fig. 5. Temperature dependence of transition strengths of absorption processes below the bandgap for pure c-Si.

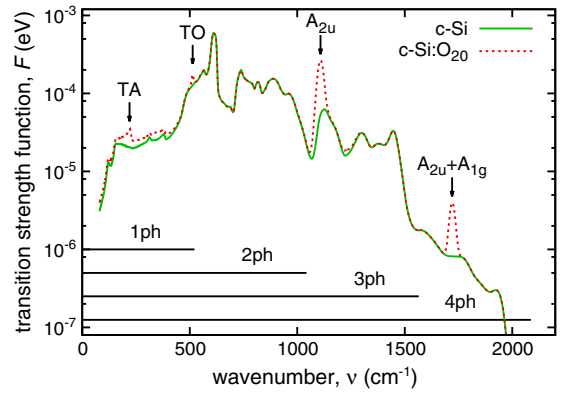


Fig. 6. Comparison of transition strength function of pure c-Si (full line) and c-Si with 20 ppm of interstitial oxygen (dotted line) at room temperature.

The relative transition strength at room temperature is  $\alpha_{A_{2u}+A_{1g}}(300\text{ K}) = 0.0025$ .

In addition to oxygen's own vibrational modes the presence of O<sub>i</sub> enhances the absorption band in the region of one-phonon Si modes (0–520 cm<sup>-1</sup>) due to locally broken symmetry of the Si crystal. Two sharp structures corresponding to the transversal acoustic (TA) and transversal optical (TO) modes are marked in Fig. 6. Their integral transition strength can be written as follows

$$N_{1ph} = \alpha_{1ph} \frac{2f_{O_i}}{1-f_{O_i}} N_{Si}, \quad (34)$$

where the relative transition strength  $\alpha_{1ph} = 0.0172$  is related to the two Si atoms closest to the interstitial oxygen atom. It is temperature independent because the absorption processes are one-phonon.

## 5. Conclusion

Parametrization of the transition strength function is a suitable starting point for the construction of dispersion models because the sum rule for transition strength function can be derived without any approximation in frame of non-relativistic quantum mechanics. It was shown how to distribute the total transition strength, i.e. the right hand side of sum rule, into individual absorption processes occurring in crystalline silicon containing interstitial oxygen. Individual dispersion formulas were not discussed but the dependences of integral transition strength of individual processes on temperature and concentration of interstitial oxygen were presented. Since some contributions depend on temperature explicitly while other only through thermal expansion the latter were described using temperature independent effective numbers of electrons or relative transition strengths. Interstitial oxygen influences the dielectric response only in the region of the phonon absorption where one-phonon absorption structures, which are not present in pure c-Si, appear. The dispersion model constructed on the basis of distribution of the total transition strength can be then parametrized using only temperature and atomic fraction of interstitial oxygen. The specific transition strength functions describing individual absorption processes will be published in forthcoming papers together with analyses of experimental ellipsometric and spectrophotometric data.

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