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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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A R T I C L E I N F O

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A B S T R A C T

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 ε_i as follows

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

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

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

where e, ϵ_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^{-1}) 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_e electrons can be written as [10]

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

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

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

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

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

The same TRK sum rule can be also written for nuclei

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

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_n and m_n 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):

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

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_i 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_r is the real part of conductivity. The linear dielectric response is then given as the sum of damped harmonic oscillators (DHOs):

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

where N_j, $E_{c,j}$ and B_j are the transition strength, central energy and broadening of DHO, respectively. The quantity N_j has unit eV^2 and is also often called oscillator strength even though it differs from unitless quantity f_{if} occurring in Eq. (3). In formula (10) the terms satisfying inequality $E_{c,j} > B_j$ can be rewritten by the Lorentz functions:

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

where E_j is the energy of transition related to the central energy of DHO by relation $E_{c,j}^2 = E_j^2 + B_j^2$.

Note that classical systems with parameters $E_{c,j} < B_j$ (overdamped oscillators) or $E_{c,j} = 0$ (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 $B_j \to 0$. 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_j is the transition strength of an individual transition $i \to j$ corresponding to absorbed energy $E_j = E_f - E_i$ 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_{ex} 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.

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