Optical analyses of radiation effects in ion-implanted Si: Fractional-derivative-spectrum methods

Xing-Fei He,* Ren-Rong Jiang, and Dang Mo
Institute of Microelectronics, Zhongshan (Sun Yat-Sen) University, Guangzhou 510275, Guangdong, People's Republic of China
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Fractional-derivative spectra (FDS) have been developed for studying radiation effects in crystals by monitoring the optical interband transitions at critical points. Optical spectra of E_1 structure of As^+-implanted Si, at doses from 3×10^{12} to 1×10^{16} ions cm^{-2}, have been analyzed with use of $\frac{3}{2}$th-derivative spectra. Symmetric line shapes in the E_1 region near 3.4 eV were found in the FDS both for crystalline and ion-implanted samples until the critical dose, above which the spectra became structureless. No change was determined, within the experimental errors, either in the line-shape symmetry or in the E_1 critical-point threshold for the implanted samples, compared with those of crystal Si, but a sharp increase in linewidth was observed. The FDS peak-to-peak height, which describes the crystal damage in the implanted region, is related to the *fractional number* of dangling bonds, found to vary with $1-(\Phi_d/\Phi)^\beta$, where $\beta\approx0.33$ initially followed by a transfer to 0.78 until saturation, Φ is the total dose, and Φ_d is a constant. Both of the sharp changes in linewidth and in dependence of the number of dangling bonds take place at the dose of 3×10^{13} ions cm^{-2}, attributed to the accumulated stresses in the damaged region. The relationship between dangling bonds and structural disorder is discussed. For annealed samples, FDS directly yielded a shrinking of the E_1 threshold, together with a decrease in the optical response. They were found to be logarithmically dependent on impurity concentration.

I. INTRODUCTION

When a heavy ion travels in a nonchanneling (random) direction in a crystal, displacement defects are produced in the wake of the implant, resulting in structural disorder or even amorphization of the bombarded crystal.[1] In such cases, it is well known that the lattice disorder builds up with ion dose until a continuous amorphous layer is formed near the surface. Annealing of the implanted sample normally leads to recrystallization of the radiation damage, but residual effects still exist due to point defects, lattice strain, or substitutional impurity atoms in the regrown region.[2] Breakdown of crystalline periodicity in the implanted material gives rise to prominent effects in electronic optical spectra, particularly in the destruction of sharp features associated with higher-edge interband transitions. This has recently received increasing attention.[3,4] Considering the relationships between interband optical properties and lattice structure, one can characterize the crystal order-disorder transformation using modulation or ellipsometry techniques,[3-6] from which the first, second, or third differential optical spectra can be obtained experimentally or numerically near Van Hove singularities. Analysis of the spectral line shapes provides information on critical-point structures,[7,8] and this has become a powerful method in studies of the electronic properties of bombarded crystals.

In this paper, we develop the method of fractional-derivative spectra[9,10] (FDS) for studying radiation effects in crystals and report on an optical study of ion-implanted Si using $\frac{3}{2}$th-derivative line-shape analyses, which yielded quite interesting information. It has been demonstrated that the $(d/2)$th derivative of a dielectric spectrum near a d-dimensional critical point has a symmetric line shape and its extremum or zero-point position corresponds to the critical-point threshold.[9] For single-crystal Si (c-Si), the E_1 structure at 3.4 eV is attributed to multiple transitions along the Λ direction in the Brillouin zone.[11,12] In spite of its complex origin, the study of the FDS for E_1 transitions presumably with $d=3$ has added to our understanding of implantation effects in the crystal. Symmetric line shapes in the E_1 region were found in the FDS both for crystalline and ion-implanted Si. Moreover, although the amplitude of FDS drastically falls with increasing crystal damage, no change was observed, within the experimental errors, in either the line-shape symmetry or in the E_1 critical-point threshold for implanted samples, until the dose reached the critical value where the spectra became structureless. However, an abrupt increase in linewidth was observed at the dose of $\Phi_0\approx3\times10^{13}$ ions cm^{-2}. Being related to the number of dangling bonds, and found to be a power function of implant dose with a transfer of power value at Φ_0, the peak-to-peak value of the FDS provides an acceptable measure of the crystal damage in the implanted region. After thermal annealing, the FDS indicated a red shift of the E_1 critical-point energy, as well as a decrease in the optical response, which are logarithmically dependent on impurity concentration.

II. FRACTIONAL-DERIVATIVE-SPECTRUM METHODS

The $(d/2)$th derivatives of the interband dielectric function, $\epsilon(E)=\epsilon_1(E)+i\epsilon_2(E)$, and its derivatives near a d-dimensional critical point were found to be,[9,10] whether d is integral or fractional,

$$E^{-2}\frac{d^{d/2}}{dE^{d/2}}[E^2\epsilon^{(k)}(E)]=\frac{i^r M_d}{E^2}\frac{k!}{(E_g-E-i\Gamma)^{k+1}}\ , \tag{1a}$$

or

$$\frac{d^{d/2}}{dE^{d/2}}[\epsilon^{(k)}(E)]=i^r A_{d,k}\frac{1}{(E_g-E-i\Gamma)^{k+1}}\ , \tag{1b}$$

when $E\approx E_g$, where

$$M_d=2|\langle v|\mathbf{a}\cdot\mathbf{p}|c\rangle|^2(e/m)^2(m_{vc}/2\pi)^{d/2}\hbar^{2-d}/\epsilon_0\ ,$$

where $A_{d,k}=k!M_d/E_g^2$. E, E_g, and Γ are the photon energy, the band gap at the critical point, and the broadening parameter describing the finite-lifetime effect, respectively, r is the type of critical points, $k=0,1,2,3,\ldots$, and $d^q f(x)/dx^q$ denotes the qth differintegral ($q>0$ for derivative and $q<0$ for integral) of $f(x)$ between the limits 0 and x.[13] The amplitude $A_{d,k}$ is proportional to the optical strength of the harmonic oscillator, f_{HO}. Presented on the right-hand sides of Eqs. (1a) and (1b) are standard Lorentzian line shapes and their kth derivatives, which are symmetric with respect to E_g.

A. Analysis of crystal amorphization

In a bombarded crystal, the implant ions create displaced atoms in the implanted area and render part of the solid into a disorder state during implantation. Because of the dangling bonds, electrons in the disorder regions do not participate in critical-point optical transitions. The optical response of a bombarded crystal, therefore, only reflects the contributions from the undamaged bonds, resulting in a decrease in critical-point optical features. Being related to the harmonic-oscillator strength,[14] and the number of dangling bonds as well, peak-to-peak height of FDS is a measure of radiation damage in the crystal.

In addition, radiation damage not only reduces the amplitudes of the optical spectra, but possibly alters the line-shape symmetry as well. The latter is due to the possible change in the degree of anisotropy of the remaining crystalline state as the amorphization process could involve directional correlations.[15] If this happens, the embedded crystallites in the damaged area will change their dimensionality compared with the undamaged crystal structure. The consequent change in the optical line-shape symmetry can be quantitatively determined by the change in parameter d in Eq. (1a) or (1b), in comparison with that in the FDS of the unimplanted crystal. With differentiation to various fractional orders on the dielectric function near a critical point, a symmetric line shape, a Lorentzian, or its derivative appears when the derivative order is equal to half of the dimension of a solid, $d/2$, as formulated in Eqs. (1a) and (1b). Therefore, the dimension of a solid, in general being fractional, is straightforwardly determined from the derivative order that yields symmetric line shapes in FDS. This dimensionality reflects the anisotropy of the remaining crystallites in the bombarded crystal.

B. Determination of critical-point parameters

Besides determining the dimension or anisotropy, the FDS also provide a direct method for measuring critical-point parameters, which is the main goal of modulation spectroscopy. In modulation spectra, e.g., wavelength-modulation absorption, $\Delta\epsilon\sim d\epsilon/dE$, or electroreflectance spectra, $\Delta\epsilon\sim d^3\epsilon/dE^3$, the line shapes generally are not symmetric. Therefore, determining E_g and Γ is somewhat complicated and special techniques, such as the three-point method[16] and Fourier transformation,[17] were required for this purpose. Using FDS, however, E_g is easily determined for a single critical point for it corresponds to either the extremum or zero point in the resulting symmetric line shape. Due to the resultant symmetric profiles, the critical-point parameters are well estimated even without use of the line-shape-fitting procedure.

III. THE $\frac{3}{2}$th-DERIVATIVE SPECTRA OF E_1 TRANSITIONS IN As^+-IMPLANTED Si

p-type silicon single-crystal $\langle 100\rangle$ wafers, with resistivity of 7–8 Ω cm, were implanted at room temperature with As^+ ions at an energy of 150 keV and to doses ranging from 3×10^{12} to 1×10^{16} ions cm^{-2}. All samples were tilted 7° off the orientation in the implantation so as to eliminate channeling effects. Thermal annealing was performed at 700 °C for 30 min in a dry N_2 atmosphere to reduce surface contamination. In order to minimize natural oxides, all samples were rinsed carefully with methylbenzene acetone ethanol $1HF:9H_2O$ mixture and then with water prior to optical measurements. Optical spectra were measured by spectroscopic ellipsometry,[18] the polarized light being set at an angle of incidence of 70°, and ellipsometric spectra obtained by analyzing the azimuth dependence of the intensity transmitted through the analyzer. The penetration depth of As^+ ions ($\sim$1400 Å) was effectively infinity in comparison with that of light in Si (400–500 Å), as discussed in our previous work,[19] so that dielectric functions $\epsilon(E)=\epsilon_1(E)+i\epsilon_2(E)$ were obtained simply using a two-phase (ambient-substrate) model.[18] The $\frac{3}{2}$th-derivative spectra of the E_1 structure for As^+-implanted Si as well as c-Si were calculated from dielectric functions using the modified Grünwald algorithm.[13]

A. Structural order-disorder transformation

The $\frac{3}{2}$th-derivative line shapes (see Fig. 1), compared with those of c-Si, remain symmetric with the same critical-point threshold, for samples at doses from 3×10^{12} up to 1×10^{14} ions cm^{-2}. However, their structures finally vanish at 1×10^{15} ions cm^{-2} when the surface had been rendered completely amorphous. During implantation, heavy As^+ ions produced defect clusters around their trajectories in collision cascades. As the bombardment dose built up, the disorder zones steadily increased in number until eventually overlap occurs, resulting in a continuous disordered layer.[20] This amorphization effect on FDS, as exhibited in Fig. 1, yields a gradual decrease of the E_1 structure without changing the

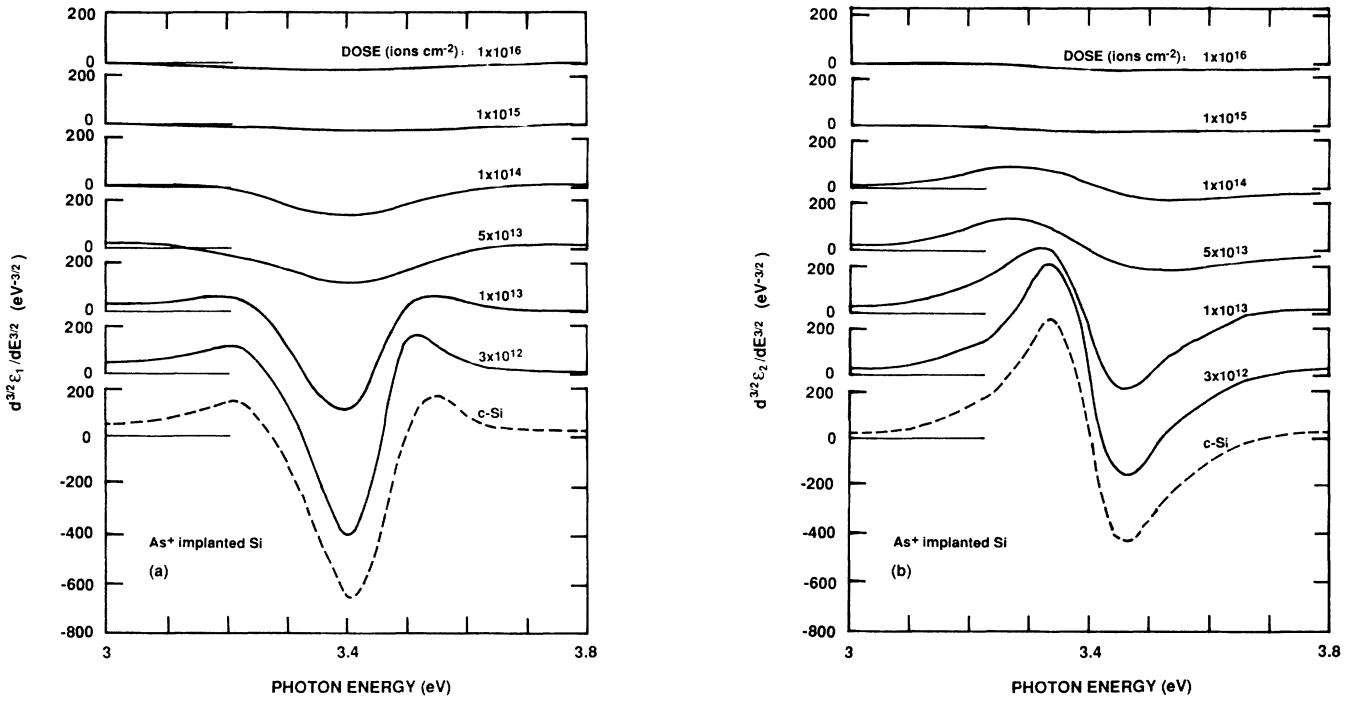

FIG. 1. The $\frac{3}{2}$th-derivative spectra in the E_1 region for c-Si (dashed lines) and for 150-keV As^+-implanted Si at doses from 3×10^{12} to 1×10^{16} ions cm^{-2} (solid lines), calculated from the dielectric functions using Eq. (1b). (a) Real parts and (b) imaginary parts.

line-shape symmetry or the critical-point energy. Some of these features were also noted by other authors in optical[3,21] and electron paramagnetic resonance[22,23] (EPR) measurements, the latter being carried out by monitoring the intensity of the EPR line at $g=2.006$.

In implanted Si which failed to reach a completely amorphous state, disorder clusters were created and distributed throughout the damaged region. Despite the breakdown of crystal periodicity in such a crystal-amorphous two-phase mixture layer, crystalline characteristics still appear in the optical spectra. This indicates that crystalline optical features remain as long as the crystalline regions exist whose dimensions are larger than the size of the excitation. Compared with those of c-Si, the unchanged line-shape symmetry in the FDS of implanted samples reveals that the amorphization of c-Si induced by ion implantation was *an isotropic process* in which neither distribution nor orientation of the displaced atoms has any directional preference emerging from the statistics. Silsbee[15] pointed out earlier that the ordered atomic array could impose directional correlations on successive collisions and that energy and momentum could be focused into those directions consisting of close-packed rows of atoms. It is expected that whenever the energy of the cascade falls below the focusing energy, the random multiplication process ceases and such focused collision sequences take place in certain low-index directions. This would cause a higher degree of disorder in some crystal orientations than others or, alternatively, the degree of crystal order in some orientations remains higher than in other directions. The anisotropic order arrangement or *the low-dimensional crystallites* embedded in the implanted region should, in fact, alter the line shapes of the FDS,[10] compared with those of c-Si. However, this was not evident in our experiment, and a more detailed analysis is required.

Although the line-shape symmetry remains unchanged throughout, an abrupt increase (by a factor of 2) in the linewidth [half-width at half maximum (HWHM)] was observed at a dose of about 3×10^{13} ions cm^{-2} (see Fig. 2). (The linewidths at doses of 1×10^{15} and 1×10^{16} ions cm^{-2} have poor accuracy.) This probably originated from the accumulated stresses within the implanted layer due to the structural change. The disorder clusters accommodated in the implanted region may introduce internal stresses to the remaining crystallites and consequently may affect the lifetime of interband transitions. Similar results were observed by Piller *et al.*[24] in their study of electroreflectance of deposited disordered Ge films, in which order-disorder transition was achieved by reducing the substrate temperature. They observed a slight increase in linewidth of $E_0+\Delta_0$ structure, when the substrate temperature dropped below 200 °C. Other nonlinear effects in the disorder-dose relationships were also noted by other authors[25] in Pb-implanted Si. They noted an abrupt increase in as-implanted dechanneling levels and remnant disorder following annealing, which they interpreted in terms of internal stresses due to the accommodation of a significant concentration of Pb impurity. In our experiment, no nonlinear responses were observed after annealing and the size of an As atom is almost the same as that of Si. Accordingly, the mechanism responsible for the linewidth increasing is mainly due to the internal stresses introduced by structural change.

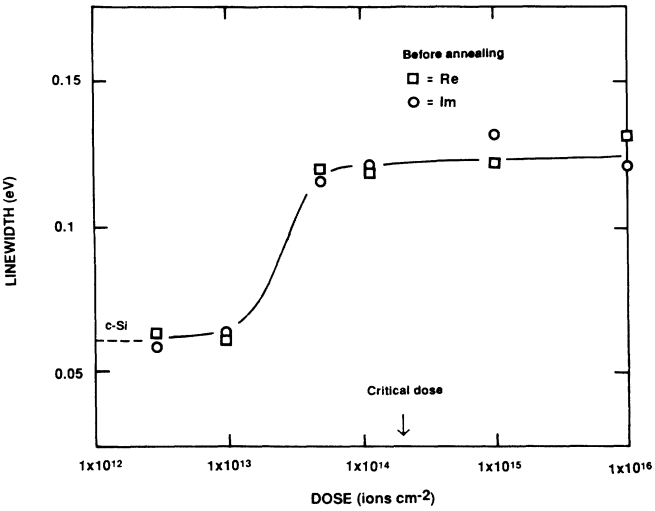

FIG. 2. The linewidth (HWHM) of the $\frac{3}{2}$th-derivative spectra. There is an abrupt increase at a dose of about 3×10^{13} ions cm^{-2}. The critical dose measured previously (2×10^{14} ions cm^{-2}) is also indicated (arrow).

B. Dangling bonds

The peak-to-peak height of FDS, $(\epsilon_1^{(3/2)})_{p\text{-}p}$ or $(\epsilon_2^{(3/2)})_{p\text{-}p}$, (see Fig. 3), which is related to the optical strength of harmonic oscillators,[14] drastically decreases with the total dose, manifesting itself as a measure of the crystal damage. Figure 3 clearly shows a critical dose, above which the crystal was changed almost to complete disorder, when the optical structure disappears. The critical dose for As^+-implanted Si measured elsewhere[20] was about 2×10^{14} ions cm^{-2} (also indicated in Fig. 3), in good agreement with our own result determined from the spectral response of the E_1 threshold. For heavy-ion implantation, cascade collisions occur in the crystal when the energy of a recoil atom is much greater than the threshold of lattice displacement. Consequently, amorphous zones are formed in the trail of a heavy implanted ion. In the case of a light ion, however, the damage is mainly in isolated interstitial-vacancy pairs. Therefore, although crystal damage builds up with bombardment dose for both heavy- and light-ion implantations, their mechanisms for structural transition are different.[26] The degree of disorder defined in effective-medium theory,[27] which was used widely to characterize the crystal damage with optical spectroscopy, describes the fractional volume of amorphous phase. It has an explicit picture only for heavy-ion implantation, where both crystal and amorphous phases coexist in the implanted layer. The damage rate determined by optical spectra, on the other hand, is related to the number of *dangling bonds* in the damaged region. This approach rests on a somewhat more microscopic point of view. The existence of amorphous zones means that an optical measurement is sampling a material with a large number of dangling bonds in the atomic mismatch regions or at the internal surfaces of the clusters.[28,29] It is these dangling bonds that render the crystal *inactive* in optical transitions, which are known as the major effect of covalent bond structure. As the amplitude of FDS is associated with the optical strength of harmonic oscillators, $[\epsilon_1^{(3/2)}]_{p\text{-}p}$ or $[\epsilon_2^{(3/2)}]_{p\text{-}p}\sim f_{HO}/\Gamma$, the peak-to-peak height of FDS for ion-implanted Si provides information on the number of bonds which are optically active or not damaged during the implantation. This is similar to the picture interpreted in EPR measurements where the signals otherwise arise from dangling bonds or unpaired electrons.[22,23]

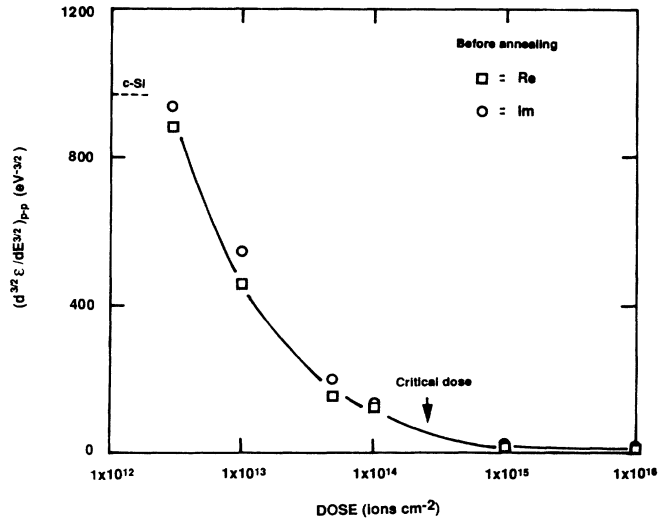

FIG. 3. The peak-to-peak heights of the $\frac{3}{2}$th-derivative spectra, drastically decreasing with crystal damage in the implanted region.

It was found that the oscillator strength has an approximate dependence on the ion dose, $f_{HO}\propto\Phi^{-\beta}$, where Φ is the dose before the occurrence of saturation and β was found to be approximately 0.33 initially, followed by a transfer to 0.78 at the dose of 3×10^{13} ions cm^{-2} (see Fig. 4), the same value at which an abrupt change in linewidth was observed. Because f_{HO} is related to the number of undamaged bonds in the implanted region,

$$f_{HO}=1-N_d\ , \tag{2}$$

where N_d is the fractional number of dangling bonds. It can be concluded that the fractional number of dangling bonds produced by the energetic implanted ions is

$$N_d=1-(\Phi_d/\Phi)^{\beta}\ ,$$
$$\beta\approx0.33\ (\Phi<\Phi_0)\ \text{and}\ \beta\approx0.78\ (\Phi>\Phi_0)\ , \tag{3}$$

where $\Phi_0\approx3\times10^{13}$ ions cm^{-2} and Φ_d is a constant. This result is different from that concluded by Lue and Shaw.[4] The authors used the relative change in reflectance derivative as a phenomenological measure of damage, while here we monitor the dielectric response theoretically corresponding to oscillator strength.

In the work of Chadderton,[30] the nucleation of damage clusters during ion implantation of Si was analyzed in detail. It was demonstrated that the disorder probed by the Rutherford scattering and/or standard channeling technique is proportional to $\Phi^{0.5}$, followed by a smooth

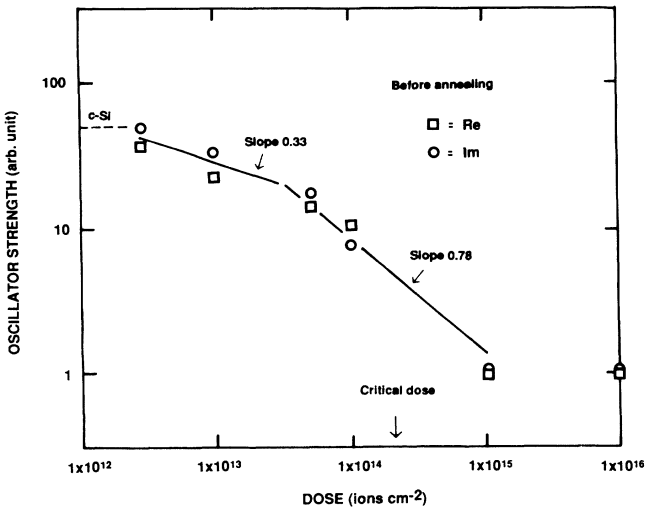

FIG. 4. Oscillator strength vs total dose, found to vary approximately with $\Phi^{-\beta}$ (solid lines) where initially $\beta \approx 0.33$, followed by a transfer to 0.78 at a dose of 3×10^{13} ions cm^{-2}; Φ is the dose before saturation.

transfer to a linear dependence before saturation finally occurs. These dependencies were proved to be shifted to lower and higher doses, respectively, by the increases in ion mass and temperature. Experimentally, it has so far almost been observed in the implantation at room temperature of heavy ions into Si that the disorder, drawn from Rutherford scattering data, is linearly dependent on dose. The disorder-dose dependencies determined using FDS are similar to those predicted theoretically by Chadderton except for the different power forms. Although the relationship is not well understood between the damage rates drawn, respectively, from Rutherford scattering and from optical response—the former being a measure of the number of interstitial defects but the latter of the number of dangling bonds—it may be concluded from the different powers (0.5 and 0.33; 1 and 0.78) that the channeling is "toughly" sampling the defect population while the optical technique is "gently" measuring the bulk reaction.

As to the change in disorder dependence, Chadderton showed, as viewed from the interactions of interstitials with the traps in the crystal, that during the periods of nucleation and primary growth small interstitials behave as unsaturable traps (homogeneous nucleation), mainly yields a $\Phi^{0.5}$ dependence, and for higher doses there is a transfer to the period of secondary growth (heterogeneous nucleation), in which the clusters behave as nucleation traps and the disorder varies linearly with ion dose until the saturation finally takes place, when the nucleation traps become saturable ones. In channeling experiments, disorder is defined as the mean number of scattering events per particle in the aligned analyzing beam, i.e., the interstitial population in the implanted crystal. On the other hand, disorder measured by optical techniques reflects the number of bonds "damaged" due to the structural transformation. It is a problem that no one really knows how the dangling bonds are created and related to the disorder structure in the implanted region. Nevertheless from the abrupt decrease in the lifetime of electronic transitions associated with the sharp change of dangling-bond dependence, it is suggested that the heterogeneous nucleation is responsible for the increase of internal stresses and consequently shortens the lifetime of E_1 transitions.

C. Impurity and free-carrier effects

After annealing, the $\frac{3}{2}$th-derivative spectra have recovered the characteristics of c-Si—sharp E_1 structure—except for a shrinkage in the threshold, $\Delta E_g = E_{g\,c\text{-Si}} - E_g$, together with a decrease in the optical response (see Fig. 5). However, no abrupt change was observed in either linewidth or oscillator strength in the corresponding region where sharp changes were determined before annealing. The shift of the E_1 energy was measured straightforwardly from the changes of positions of the minima in the real parts, $\Delta[\epsilon_1^{(3/2)}]_{\min}$, and the zero point in the imaginary parts, $\Delta[\epsilon_2^{(3/2)}]_{\text{zero}}$, of FDS, though the extremum or the zero point itself certainly does not correspond to the critical-point energy due to E_1 complex transitions. Both of the residual effects were found to increase with implant dose. The shift of the E_1 threshold measured by line-shape fitting using the first differential spectra—as in our previous work[31]—is also plotted in Fig. 5 for comparison. They are in reasonable agreement. Electrical measurements[32–34] on As^+-implanted and annealed Si at conditions fairly similar to those in our experiments indicated that after annealing a

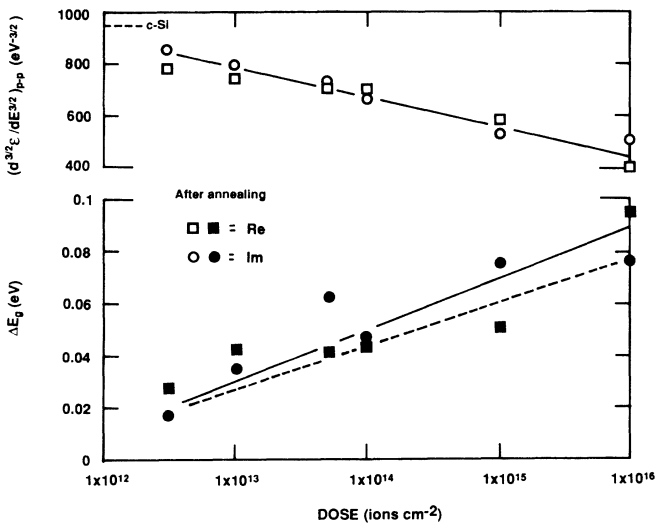

FIG. 5. The red shift of the E_1 threshold and the decrease in the peak-to-peak value of the $\frac{3}{2}$th-derivative spectra due to the substitutional impurities and the screening of free carriers after annealing. The shift of the critical-point energy, found roughly proportional to $\gamma \log\Phi$ ($\gamma = 0.02$ eV), was measured directly from the changes of the minimum and zero-point positions in the fractional-derivative spectra (solid line), and compared with that determined by first-derivative line-shape fitting (dashed line) in our previous work.

large fraction of As atoms is electrically active, i.e., most impurities are on substitutional sites. Taking into account the fact that arsenic is nearly the same size as silicon, one may expect the lattice strain induced by the impurities to be negligible. The residual effects, therefore, are due mainly to the substitutional impurities and the screening of free carriers released by the As atoms.

One of the main effects of component disorder induced by impurities is to shift critical points to lower energies. Vinã and Cardona[5] observed a red shift of the E_1 critical point in ion-implanted and annealed Si using the third differential spectrum analysis. They fitted the shift to the function of impurity concentration, $\sim n^{0.46}$, for the E_1 critical point compared with the theoretical dependence $n^{0.5}$ obtained by their perturbation-theory calculations of the change in the band structure of Si due to randomly substitutional impurity potentials. However, Aspnes *et al.*[35] concluded, also based on line-shape fitting, that the threshold varied approximately linearly in n, which was predicted by Allen and co-workers[36–38] as a result of an ensemble average over form and structure factors for random impurity atoms. In addition, Berggren and Sernelius[39] showed that electron-electron interactions produce a shift proportional to $n^{1/3}$ while screened electron-ion interactions provide an $n^{1/2}$ dependence for the fundamental indirect gap of Si. Our experimental data were found to be consistent with a linear slope (0.02 eV) in semilogarithmic coordinates (Fig. 5), i.e.,

$$\Delta E_g = \gamma \log(\Phi/\Phi_c), \quad \gamma = 0.02 \text{ eV} \tag{4}$$

where Φ_c is a constant (approximately 3×10^{11} ions cm^{-2}). In the first-order approximation the average impurity concentration n and dose can be related by[40] $n \approx 0.2\Phi/\Delta R_p$ and $n_c \approx 0.2\Phi_c/\Delta R_p$, where ΔR_p is the standard deviation in the projected range ($\Delta R_p \approx 30$ nm in our experiment). Substituting the expression into Eq. (4) gives the shift of critical-point energy as a function of n,

$$\Delta E_g = \gamma \log(n/n_c), \quad \gamma = 0.02 \text{ eV} \tag{5}$$

where $n_c \approx 2\times10^{16}$ cm^{-3}. The impurity concentration in this work is approximately in the range 2×10^{17}–7×10^{20} cm^{-3}. Although the dependency concluded here is different from that obtained by Vinã and Cardona,[5] the total shift of the critical-point threshold measured by FDS is almost the same as that in Ref. 5 ($\Delta E_g = 0.002$–0.09 eV) in the same concentration range.

As to the blurring of the E_1 peak, a similar effect has been observed in the previous work,[5,35,41] and was attributed to the screening of excitonic interaction by free carriers. The Thomas-Fermi screening length for Si (Ref. 39) is proportional to $n^{-1/6}$, decreasing with doping concentration. If the exciton radius for a given critical point is larger than the screening length, then the sharp excitonic structure for that critical point should disappear in the optical spectra.[42] The decrease in the optical response, $(\Delta\epsilon_1^{(3/2)})_{\text{p-p}}$ or $(\Delta\epsilon_2^{(3/2)})_{\text{p-p}}$, was also found roughly to be a logarithmic dependent on dose or impurity concentration.

IV. CONCLUSION

As can be seen, the FDS methods have advantages in line-shape analyzing and directly yielding critical-point thresholds. Symmetry analysis in FDS of dielectric functions provides information on the anisotropy of the amorphization process in a bombarded crystal. Although the damage depth profile should be taken into account in a more detailed analysis,[43,44] the peak-to-peak height of FDS provides a measure of the degree of disorder since it is related to the number of dangling bonds in the damaged area. This picture is microscopically suitable for both heavy- and light-ion implantations. With FDS, a critical-point threshold can be easily determined even without line-shape-fitting procedures.

Optical structure of E_1 transitions of As^+-implanted Si was analyzed using $\frac{3}{2}$th-derivative spectra. Unchanged line-shape symmetry and a sharp increase in linewidth were observed in the FDS. The fractional number of dangling bonds in the implanted region was found to be a $1-(\Phi_d/\Phi)^\beta$ dependence, where initially $\beta \approx 0.33$, followed by a transfer to 0.78 until saturation. Both of the sharp changes in linewidth and dangling-bond dependence took place at a dose of 3×10^{13} ions cm^{-2}, and are attributed to the internal stresses in the implanted region. FDS of annealed samples directly yielded a red shift of E_1 threshold and a decrease of optical response, which are logarithmically dependent on impurity concentration.

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*Present address: Laser Physics Centre, Research School of Physical Sciences, Institute of Advanced Studies, Australian National University, G.P.O. Box 4, Canberra, Australian Capital Territory 2601, Australia.

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