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On the origin of resonance features in reflectance difference data of silicon

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Abstract

The physical origin of sharp resonances in reflectance difference spectroscopy (RDS) data at the critical points of the dielectric function of bulk Si, previously assigned to surface-bulk transitions, to photon localization or to optical transitions from bound dimer states to excited dimer states is investigated. We show that uniaxial in plane stress of bulk Si induces sharp resonances at exactly these critical points of Si via the piezo-optic effect. In the recent literature, it was shown that surface reconstruction as well as dimerization exerts anisotropic stress, e.g. along the dimer direction, and the resulting strain is extending into the bulk. In our contribution, we simulate this surface strain by externally stressing different Si faces and compare ex situ measured RDS data of Si(0 0 1), Si(1 1 1) and Si(1 1 0) surfaces with RDS data measured in situ and density functional theory calculations. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

A continuing goal of epitaxial crystal growth is the production of high quality material and atomic control of surfaces. In situ monitoring techniques such as reflectance difference/anisotropy spectroscopy (RDS/RAS) are extremely helpful to reach this target.

RDS measures the difference in reflectance between two orthogonal polarizations [1]. RDS is now an established diagnostic tool for monitoring surface processes. However, the origin of surface induced optical anisotropy (SIOA) features in RDS data is still not completely understood. Much of the experimental work has concentrated on III–V [2,3] and II–VI [4,5] surfaces. The applicability of RDS to Si is somewhat limited, however, because of the lack of a satisfactory correspondence between the experimental SIOA of Si(1 1 1) [6] and Si(0 0 1) surfaces [7,8,9] and atomic models [10,11,12,13].

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It is usually argued that the RDS response of bulk is nominally isotropic for zincblende and diamond semiconductors, therefore any observed optical anisotropy shall be surface induced. The main discrepancies between density functional theory (DFT) calculations and measurements are occurring at the critical points of the dielectric function of bulk silicon. The fact that RD spectra have a large magnitude at the energies of critical points of the bulk dielectric function (and are often similar to its energy derivative) supported expectations that surface states are of minor importance for the origin of these particular features.

The purpose of this contribution is to point out the possibility that some of the observed features on reconstructed Si surfaces are strain-induced effects, where the stress as driving force is occurring due to surface reconstruction, steps or dimerization. That dimerization induces *anisotropic* stress was found experimentally with scanning tunneling microscopy in [14,15] and was theoretically predicted in [16]. Comparing the ex situ data presented here with in situ data published earlier a good agreement in the SIOA structures is found. Therefore, we conclude that part of the SIOA is arising from anisotropic strain fields, which are building up when dimerization, respectively, step formation at the surface occur and therefore strain-fields arise. As a matter of fact, when both domains ((2×1) and (1×2)) are present on Si(0 0 1) the average macroscopic strain cancels. Also the magnitude, as well as the spectral line shape of the real and imaginary part of the piezo-optic coefficients P_{11} , P_{12} and P_{44} [17], measured with spectroscopic ellipsometry (SE), indicate that bulk strain larger than a few MPa should be detectable with RDS, especially at the energy of the E_1 interband transition. As already pointed out in [18] the P_{44} piezo-optic coefficient can be written as a sum of the energy-derivative of the dielectric function plus a term proportional to the dielectric function.

In polar III–V and II–VI compounds one identified cause for optical anisotropy of bulk samples is the linear electro-optical effect (LEO), caused by the surface electric field due to Fermi level pinning [19]. Here it has to be mentioned that the authors of [19] implicitly make use of the converse piezo-electric effect (electric field induces a stress and strain field). This strain field splits the otherwise degenerate eight ellipsoids along the $[\pm 1, \pm 1, \pm 1]$ directions into

two sets of four and thereby modifies the bulk reflectivity for polarizations along $[\bar{1} 1 0]$ and $[1 1 0]$. This effect occurs strongest at the E_1 and $E_1 + \Delta_1$ interband transitions energy of zincblende semiconductors. The piezo-optic effect occurs not only in zincblende structures, where the origin for the anisotropic strain can also be due to the converse piezo-electric effect, but also in semiconductors with a diamond structure, where the piezo-electric effect is forbidden.

An immediate implication of our results is that slab calculations need to account for strain effects in order to calculate RDS spectra in good agreement with experiment.

2. Experimental details

In RDS the measured quantity is the difference between the normal incidence reflectances for the two orthogonal polarization directions in the surface plane. The results are displayed as $\Delta\tilde{r}/\tilde{r} = \Delta r/r + i\Delta\theta$ with $\tilde{r} = r \exp(i\theta)$. We define for (0 0 1) surfaces $\Delta\tilde{r} = \tilde{r}_{\bar{1}10} - \tilde{r}_{110}$, for (1 1 1) surfaces $\Delta\tilde{r} = \tilde{r}_{\bar{1}10} - \tilde{r}_{\bar{1}\bar{1}2}$, and for (1 1 0) surfaces $\Delta\tilde{r} = \tilde{r}_{\bar{1}10} - \tilde{r}_{00\bar{1}}$, where the suffixes denote the incident polarization vectors. The same experimental setup is used as in [2].

The anisotropic stress was applied along the following directions: $[1 1 0]$ and along $[\bar{1} 1 0]$ for Si(0 0 1), along $[0 0 1]$ and $[\bar{1} 1 0]$ for Si(1 1 0), and along $[1 \bar{1} 0]$ and $[\bar{1} \bar{1} 2]$ for Si(1 1 1). If not stated otherwise, an anisotropic stress of 25 MPa was used, which yields, slightly dependent on the Si face, a small strain of approximately 2×10^{-4} .

We compare ex situ measured RDS data of anisotropically stressed and unstressed Si(1 1 0), Si(1 1 1) and Si(0 0 1) surfaces. All these surfaces are covered with natural oxide or are immersed in 5% hydro-fluorid (HF) acid solution. The experiments were carried out at room temperature.

3. Experimental results

3.1. Si (1 1 0) surface

Fig. 1 displays the results of external stress on an Si(1 1 0) surface, which is covered with a natural

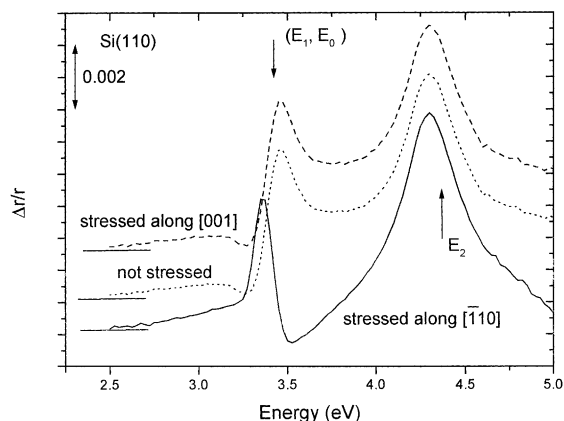


Fig. 1. RDS data Si (1 1 0); the dotted line displays the intrinsic RD spectrum for the unstressed sample, the dashed line displays the RD data taken under uniaxial stress along [0 0 1], the full line represents the RDS data taken under uniaxial stress along $\bar{1}10$.

oxide of 31 Å as determined with SE. In Fig. 1, the dotted line displays the well known RD spectrum for Si(1 1 0) surfaces without external stress [1]. It has been argued in the past that the SIOA of this face is due to a local field effect induced by the truncation of the bulk [20,21]. The other possible explanation in the literature is attributed to spatial dispersion [22]. The dashed line, vertically shifted upwards for the sake of clarity, was taken under uniaxial stress along [0 0 1]. There is no change in the line shape in comparison to the data taken without stress.

If, however, the sample is squeezed with uniaxial stress along $\bar{1}10$ with 100 MPa a change occurs. The full line represents these RDS data. Although the strain is small, a change at the E_1 and E'_0 complex is obvious. Because the E_1 and E'_0 transitions are only 70 meV apart at room temperature and can be barely resolved, these transitions are indicated on all figures by one arrow. It seems that the resonance of these transitions changed under stress to a derivative like structure of the unstressed one. At the E_2 transition the spectral shape does not change. The background however is modified.

3.2. Si (1 1 1) surface

Fig. 2 shows a comparison between six data sets taken on three different samples. Fig. 2a displays the data measured by Yasuda, et al. on Si(1 1 1):H sur-

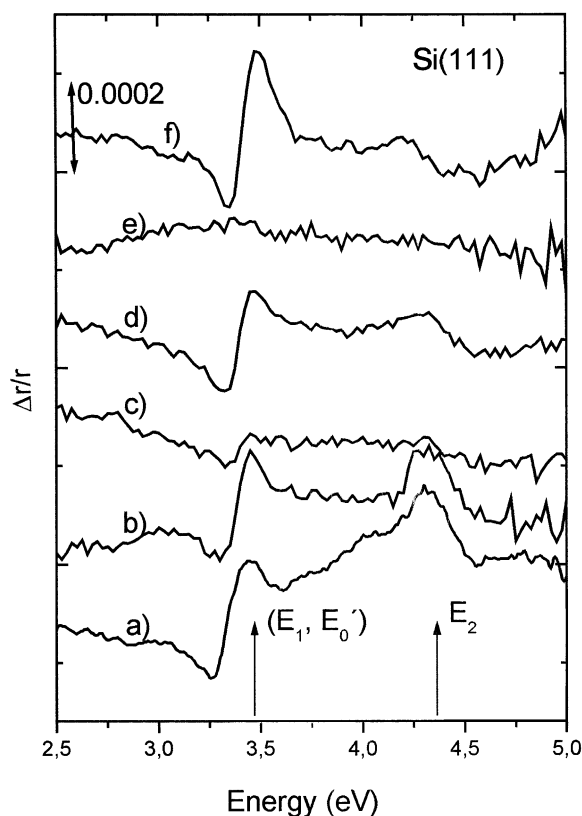


Fig. 2. (a) Displays the RD data of a Si(1 1 1):H surface 5° miscut towards the $[1\bar{1}2]$ direction, from [23]; (b) shows ex situ measured data on Si(1 1 1) surfaces covered with natural oxides and 2° miscut; (c) same as Fig. 2b with the RDS head rotated by 45° from the $[1\bar{1}0]$ direction towards the $[2\bar{1}\bar{1}]$ direction; (d) same as Fig. 2c with the application of 25 MPa compressive stress along the $[1\bar{1}0]$ direction; (e) the RD spectrum of a non miscut Si(1 1 1) sample (f) same as Fig. 2e with the application of 25 MPa uniaxial stress along the $[1\bar{1}0]$ direction.

faces with a 5° miscut towards the $[1\bar{1}2]$ direction [23]. The data exhibit two distinct SIOA features, one at the E_1 , E'_0 transitions, and the other one at E_2 . In Fig. 2b ex situ measured data on Si(1 1 1) surfaces covered with natural oxides and 2° miscut towards the $[2\bar{1}\bar{1}]$ direction are shown. Although there is a different background, the same resonances are observed as in UHV on the sample with a 5° miscut. In Fig. 2c, the RDS spectra of the same sample is shown, when the RDS setup is rotated 45° towards the $[2\bar{1}\bar{1}]$ direction. To be specific, $\Delta\tilde{r}$ is now defined as difference of reflectances along the $[-1 - \sqrt{3}, -1 + \sqrt{3}, 2]$ and $[1 - \sqrt{3}, 1 + \sqrt{3}, -2]$ directions. In Fig. 2d, the

RD response is shown in the same configuration as in Fig. 2c, but now the sample is compressively stressed with 25 MPa along the $[1\bar{1}0]$ direction. As it can be seen there is a structure at the E_1, E'_0 complex building up, very similar to Fig. 2a and b, where the same structure is present without external stress. In Fig. 2e, the RD spectrum of a non-miscut sample (actually 0.03° , as determined with high resolution X-ray diffraction) is shown. A featureless flat line results for this surface. Applying uniaxial stress along the $[1\bar{1}0]$ direction gives rise to the spectrum shown in Fig. 2f.

3.3. Si(0 0 1) surface

Fig. 3 compares in situ literature RDS data of the single domain Si(0 0 1) surfaces with ex situ RDS data of oxidized Si(0 0 1) anisotropically stressed. In Fig. 3a, a RDS spectrum at room temperature is shown, which was obtained from a single domain Si(0 0 1)

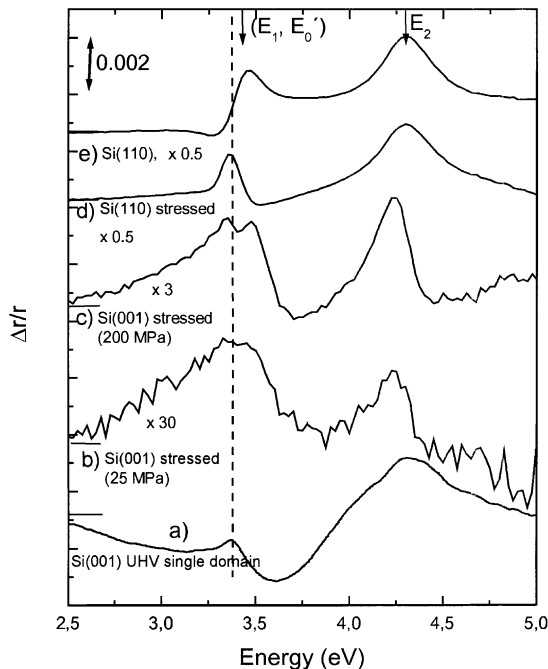


Fig. 3. (a) RDS spectrum of a single domain Si(0 0 1) surface, from [8]. (b) RDS spectrum of an oxidised non miscut Si(0 0 1) with external uniaxial stress of 25 MPa ($\times 30$). (c) Same as Fig. 3c, with 200 MPa ($\times 3$); (d) and (e) are replotted data from Fig. 1 (full line and dotted line). They are scaled with 0.5.

surface, miscut less than 0.3° from $[0 0 1]$ direction [7]. The RDS spectrum in Fig. 3b (multiplied by 30) was measured ex situ on an oxidized non miscut Si(0 0 1) under an external uniaxial stress along $[\bar{1} 1 0]$. The RD response of a non-stressed Si(0 0 1) is flat. If the stress is increased to about 200 MPa, Fig. 3c results (multiplied by 3). With increased stress the broad peak at the E_1 and E'_0 region splits into two peaks 300 meV apart. For comparison we deliberately show in Fig. 3d and e data for Si(1 1 0) surfaces with and without external stress (cf. Fig. 1a and c). The correspondence of the peaks at the E_1 and E'_0 complex, as well as at the E_2 region is evident.

4. Discussion

The dispersion of the piezo-optic data of Si were first measured by Etchegoin et al. [17] with spectroscopic ellipsometry. Using Voigt notation, the piezo-optic tensor can be written as 6×6 matrix with three independent and complex coefficients $P_{11}(\omega)$, $P_{12}(\omega)$ and $P_{44}(\omega)$. The RDS response is then calculated as pure bulk response as $\Delta\tilde{r}/\tilde{r} = \Delta\epsilon/((\epsilon - 1)\sqrt{\epsilon})$ [24]. For the three different surfaces the piezo-optical response of a bulk sample can then be calculated, assuming that the anisotropic stress directions are parallel to the crystallographic directions, given as subscripts in the RDS signal ($\Delta\tilde{r}$) for the respective surface. The stress magnitudes are denoted by $\sigma_\perp$ and $\sigma_\parallel$. For the Si(0 0 1) surface the only observable piezo-optic coefficient is P_{44} , if an anisotropic stress tensor is present with the components in diagonal form $\Delta\epsilon = P_{44}(\sigma_\perp - \sigma_\parallel)$. For the Si(1 1 1) surface the dielectric function anisotropy results as $\Delta\epsilon = (P_{11} - P_{12} + 2P_{44})(\sigma_\perp - \sigma_\parallel)/3$. For the Si(1 1 0) surface it is interesting to note, that also stress along the z direction σ_z (along $[1\bar{1}0]$) is yielding an anisotropy in the RD signal, giving in total $\Delta\epsilon = (P_{11} - P_{12})\sigma_\perp + (P_{12} - P_{11} - P_{44})\sigma_\parallel/2 + (P_{12} - P_{11} + P_{44})\sigma_z/2$. However, on a free surface stress in z direction should not be present.

Using the published piezo-optic coefficients, it is possible to describe the measured stress effects with RDS for the case of Si(1 1 1) and Si(1 1 0). For the Si(0 0 1) surface, the change of the RDS data with stress *cannot* be fitted satisfactory with the published piezo-optic coefficients.

4.1. Si(1 1 0) surface

Although the Si(1 1 0) surface even serves as calibration standard for RDS apparatus, knowledge about this surface is rather limited. Some experiments indicate that clean vicinal Si(1 1 0) surface separates into the (47 35 7) and (17 15 1) facets [25]. Facetting would most probably be driven by strain. Other experiments using scanning tunneling microscopy reveal that the elemental structure of the clean Si(1 1 0)-“ 16×2 ” is a pair of pentagons [26]. Also here it is not improbable that this reconstruction is inducing surface strain.

The comparison between the calculated piezo-optic RDS response and the measured oxidized RDS data, HF stripped and a density functional theory (DFT) calculation is shown in Fig. 4. Fig. 4a shows the reflectance anisotropy calculated from first principles for Si(1 1 1):H surface, with 5×10^{-3} compressive strain along the $[\bar{1}\bar{1}2]$ direction and 5×10^{-3} tensile strain along $[\bar{1}10]$. Our calculations employ a massively parallel, real-space finite-difference implementation of the density-functional theory in the local-density approximation (DFT-LDA). A multi-grid technique is used for convergence acceleration. The spacing of the finest grid used to represent the electronic wave functions and charge density is 0.238 Å. This corresponds to an energy cut-off in plane-wave calculations of about 24 Ry. Further details are like those in [10,13]. Without external

stress, the calculation of non-miscut Si(1 1 1):H surface does not show any optical anisotropy. We compare in Fig. 4 the two different surfaces to show, that even on a high symmetry surface optical anisotropy can be numerically obtained with DFT-LDA calculations, if the underlying bulk is strained. On the contrary, it could be, that strain, due to surface dimerization, plays a role on different faces, e.g. on Si(1 1 0). Fig. 4b and c shows the measured RDS data of oxidized, respectively HF stripped, Si(1 1 0). Assuming, that residual stress is influencing the not externally stressed Si(1 1 0) RDS data, a reasonable fit of the lineshape (Fig. 4d) can be obtained when s_z is chosen as large as $\sigma_{||}$ (200 MPa). Fig. 4d was not shifted vertically; i.e. that the high base line could be due to slight errors in P_{44} in [17] arising from oxide corrections of SE data.

That the RDS data are different, if the sample is squeezed along $[001]$ (almost no change, dashed line of Fig. 1) or along $[\bar{1}10]$ (strong change, full line of Fig. 1) can be understood by taking into account the modification of the selection rules by external stress [27]. Stress along any $\langle 001 \rangle$ direction does not lift the degeneracy of the eight ellipsoids the $[\pm 1, \pm 1, \pm 1]$ directions, whereas stress along $[\bar{1}10]$ splits the eight transitions into two sets of four. However, we are currently not in the position to draw final conclusions, because we do not know from the UHV experiments, how the strain field penetrates into the depth.

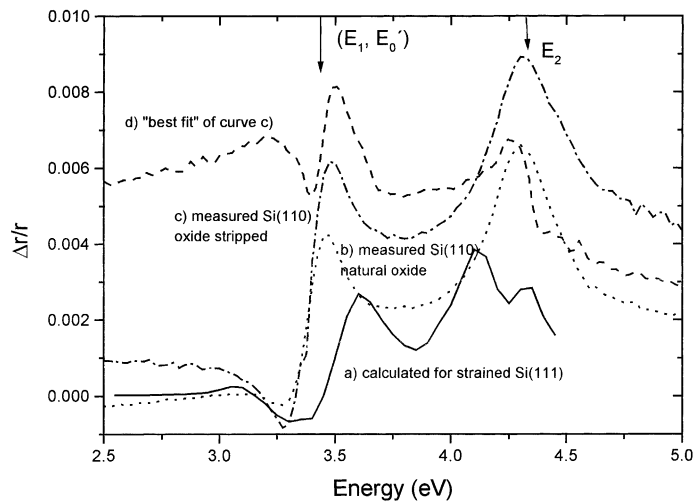


Fig. 4. (a) DFT calculation of the RD response of a strained Si(1 1 1):H surface (see text); (b) and (c) show the measured RDS data of oxidised, respectively, HF stripped, Si(1 1 0); (d) displays the best fit of Fig. 4b with published piezo-optic [17] (data not shifted vertically).

4.2. Si (1 1 1) surface

Using the published data for the piezo-optic coefficients of Si, the agreement between the measured stress effects (e.g. Fig. 2f) and the calculated response is excellent in terms of the critical points as well as in magnitude for the given anisotropic stress of 25 MPa. The dichroism for this surface depends only on the difference between $\sigma_{\perp}$ and $\sigma_{\parallel}$, as discussed above. At the E_1 and E'_0 complex the data are in good agreement with the DFT calculation of the Si(1 1 1):H surface, shown in Fig. 4a. At the E_2 transition energy, however, the DFT calculation does not agree with the measured data. This may be related to the limitations of our calculation. The neglect of excitonic effects [28] in the calculations leads to a bulk dielectric function where the E_1 peak is underestimated by about 50% and reduced to a weak shoulder of the E_2 peak [21]. Additionally, the surface local-field effect, not accounted for in our study, may influence the line shape [20]. Self-energy effects on the RDS data [29] are only approximately included via a scissors-operator [30] approach.

Although the agreement between theory and experiment is still far from satisfactory, the main conclusion

we can draw is that uniaxial stress is inducing resonances exactly at the critical points of the dielectric function. The remaining open question is, if the RD resonances as shown for H-terminated miscut surfaces in Fig. 2a or for oxidized miscut samples in Fig. 2b is due to the step contribution and to its electronic rearrangement [6,10] or due to stress induced by the steps.

4.3. Si (0 0 1) surface

As pointed out by Mönch [31] and corroborated by experiment [14] and theory [16], the dimers on the Si(0 0 1) surface stress the surface region anisotropically. This sums up to a collective effect, when the balance of the (2×1) and (1×2) domains is shifted towards a single domain surface as it is the case for surfaces prepared with electro-migration [8]. It is interesting to note, how single domain surfaces on Si(0 0 1) are prepared [7], which give an RDS spectrum as in Fig. 3a. In order to produce only one terrace type, samples are strained along the $[1 \bar{1} 0]$ directions at elevated temperatures, which lowers the free energy and thus increases the area of one terrace type with respect to the other [32]. The surface was then

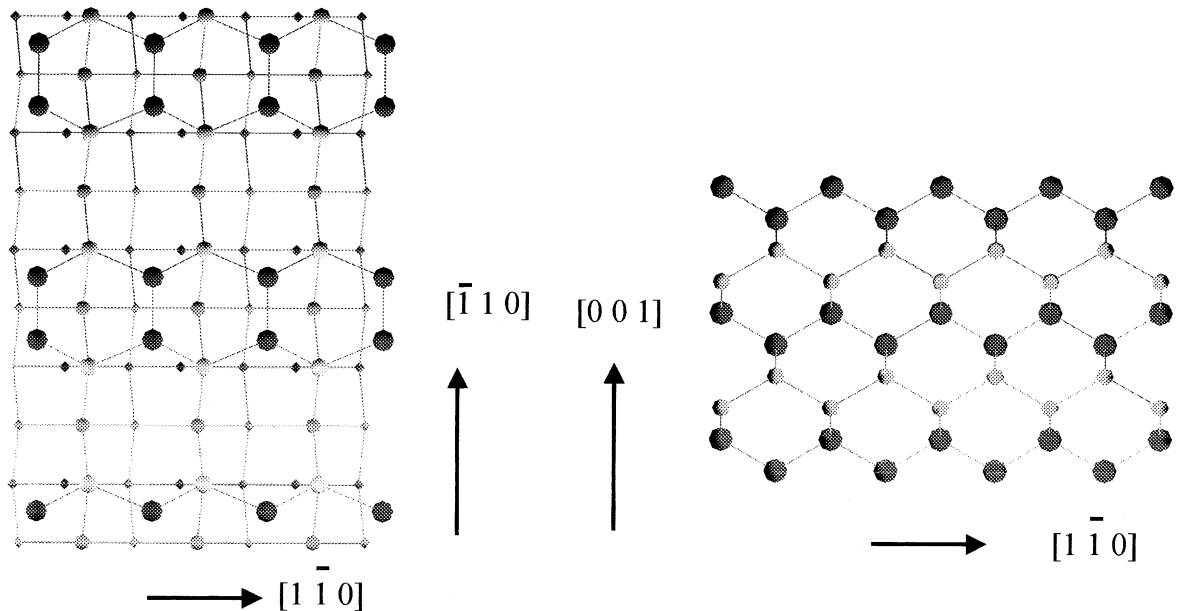


Fig. 5. (a) Top view onto the Si (0 0 1) surface; (b) top view onto the Si (1 1 0) surface.

quenched at low sample temperature before removing the *externally* applied stress, producing surfaces with the same low step density as the equilibrium surface but with high population asymmetries between the (2×1) and (1×2) terraces. Using the published data for bulk Si [17], it is not possible to fit the measured changes for the Si(0 0 1) surface, neither Fig. 3b, nor Fig. 3c, satisfactorily.

Because there is only a slight correspondence between the RDS spectrum of the weakly uniaxially stressed (25 MPa, Fig. 3b) and the strongly stressed Si (200 MPa, Fig. 3c) to the in situ single domain results (Fig. 3a), we propose a different mechanism for the origin of the resonances at the E_1 and E'_0 complex and at the E_2 critical point. The similarity between Fig. 3d (Si(1 1 0) stressed) and Fig. 3a (Si(0 0 1) single domain) led us to the conclusion, that the dimer zig-zag chain, which is present at both of these surfaces responds on the external stress in the same way. The peak at the E_1 and E'_0 complex, but also for the E_2 transition is at exactly the same position and has the same lineshape in the stressed Si(1 1 0) and in the single domain Si(0 0 1). In Fig. 5a, the top view of the Si(0 0 1) surface is shown, for the five uppermost atomic layers. The atoms, which form the dimers are also located along the zig-zag chain direction along $[1\ 1\ 0]$. The dimers are pulling together the topmost atoms on the Si(0 0 1) surface, such that light propagating in z direction probes the in-plane component of the zig-zag chain. In Fig. 5b, a Si(1 1 0) surface is shown, drawn two layers deep. Light falling perpendicular on the sample probes only the in plane component of these zig-zag chains. Due to the very good agreement between the stressed Si(1 1 0) response and the single domain UHV surface, we speculate that the dimer layer on Si(0 0 1) stresses the zig-zag chains in the same way, as it is emulated by external compressive stress on Si(1 1 0).

5. Conclusion

In this study, we have shown that uniaxial in-plane stress induces sharp resonances in RDS data at critical points of the dielectric function of the bulk semiconductor via the piezo-optic effect. Because surface reconstruction and dimerization exerts anisotropic stress, strain extends into the bulk. For the Si(1 1 1)

surface, there is strong evidence, that the RDS features seen previously can be modeled by anisotropic stress. For the Si(0 0 1) as well as the Si(1 1 0) surface, however, definite conclusions are not yet possible. Nevertheless, the influence of stress on RDS data was demonstrated also for these surfaces. When analyzing in situ RDS data in terms of surface local-field effects, surface-bulk transitions, etc. the experimental conditions shall be chosen in such a way that residual strain can be measured.

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