Surface-induced optical anisotropy of the (001) and (113) silicon surfaces

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The surface-induced optical anisotropy of clean and hydrogenated (001) and (113) surfaces of silicon has been calculated. The equilibrium atomic configurations of the surface atomic structures were determined from fully converged self-consistent total-energy calculations within the local density approximation. The optical functions of the silicon surfaces have been obtained beyond the density-functional theory with *ab initio* pseudopotentials and by the semiempirical tight-binding method. The reflectance anisotropy (RA) spectroscopy signal of the clean (001) and (113) surfaces in the region around 3.0 eV originates from surface to bulk optical transitions. On the hydrogenated (113) silicon surface a strong surface induced RA response is obtained in the region of the E_1 and E_2 bulk critical points, where the line shape corresponds to the first derivative of the bulk dielectric function. The calculated RA spectrum of the hydrogenated (113) silicon surface in the regions of the E_1 and E_2 structures is more intense in relation to the (001) surface. These results will be discussed in comparison with experimental data. [S0163-1829(98)07743-1]

I. INTRODUCTION

The surface-induced optical anisotropy (SIOA) of semiconductors has become an important tool in the study of semiconductor surfaces.[1–7] The SIOA effect originates from structural and electronic distortions due to changes in the surface geometry. Therefore, SIOA is very effective in characterizing the nature of the structural and electronic properties of semiconductor surfaces, both *in situ* and *ex situ*. Since the bulk optical response of cubic crystals with full translational symmetry is isotropic, SIOA can be observed using reflectance anisotropy (RA) spectroscopy. In this method the difference between near-normal-incidence reflectances of light polarized along two principal axes of the sample in the plane is determined. For example, in cubic materials RA spectroscopy measures the difference in light linearly polarized along the [110] and $[1\bar{1}0]$ principal axes in the plane of the (001) surface. Thus RA spectroscopy has proven to be well suited for isolating the surface optical response of cubic semiconductors. It should be pointed out that this method also has been employed to study the in-plane anisotropy produced by other effects such as near surface electric fields (zinc-blende-type materials),[8] dislocations,[9] and buried heterointerfaces.[10] However, the use of RA spectroscopy to study the SIOA in Si (as well as other materials) is currently limited by a lack of detailed understanding of the origins of the experimentally observed spectral features.[11]

The SIOA of clean and hydrogenated vicinal (001) and (113) Si surfaces measured by RA spectroscopy has been reported recently in Refs. 1, 2, 4, and 11. Chemically cleaned Si(001) surfaces, where dangling bonds were passivated either with hydrogen or with oxygen, showed sharp step-induced derivativelike features that increased with vicinal angle. The RA spectra of clean reconstructed (001) (2×1) and (113) (3×2) surfaces showed both a broad structure near 3.0 eV, which has been assumed to involve dangling bond transitions, and a second feature near 4.3 eV that corresponds to the E_2 peak of bulk Si.

The nature of SIOA could be caused by the following main contributions: changes in atomic structure on the surface as a result of the reconstruction processes;[6] local electric fields that could cause a linear electro-optical effect in Si as a result of the reduction of the symmetry on the surface and the appearance of charge transfer after the adsorption of foreign atoms on the surface (e.g., hydrogen);[8,11] anisotropic mechanical stresses due to misfit dislocations on or near the surface.[9] In the present work we have numerically calculated the SIOA of Si (001) and (113) surfaces caused by atomic reconstruction processes. We have used *ab initio* density functional theory (DFT) within the local density approximation (LDA) as well as a semiempirical tight-binding method (SETBM). Equilibrium atomic geometries of the surfaces have been obtained by the total energy minimization method. Optical functions have been calculated either by plane-wave expansion of *ab initio* pseudopotentials or by empirical parametrization of optical matrix elements. Strong surface-induced optical response is obtained in the region around 3.0 eV, which originates from surface-to-bulk optical transitions, as well as in the regions of the E_1 and E_2 bulk critical points. We show that the line shape of the E_1 and E_2 related response of the hydrogenated (113) (3×1) Si surface corresponds to the first derivative of the dielectric function of bulk Si. We discuss our results in comparison with recently available experimental data.[1,2,4,11]

II. ATOMIC GEOMETRY

As an input for the calculation of the optical functions we used atomic coordinates as determined in this work by the energy minimization method. The equilibrium atomic geometries of the clean and hydrogenated (001) and (113) silicon surfaces have been obtained in this work from fully converged self-consistent total-energy calculations within DFT-LDA. The electron-ion interaction is treated by using norm-conserving *ab initio*, fully separable pseudopotentials in the Kleinman-Bylander form.[12] To simulate the surface the

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repeated-slab method is used. The energy minimization is based on a Car-Parinello molecular-dynamics scheme. The electronic-structure calculations underlying the computations of the optical properties are based on the DFT-LDA.[13] The many-body electron-electron interaction is described within LDA, more precisely within the Ceperley-Alder scheme[14] as parametrized by Perdew and Zunger.[15] The plane-waves basis was defined by the cutoff energy of 8 Ry. To simulate the surface a 12-layer slab of Si atoms has been used, where the top 4 layers on each side were allowed to relax and remaining 4 layers were fixed at their bulk sites. We used (3×2) surface unit cell, and the electron density we calculated with 2 special $\mathbf{k}_{\parallel}$ points in the surface Brillouin zone (BZ). This formulation of the problem is close to Ref. 16 where a similar method was used. We found that without hydrogen a truncated bulk (1×1) structure relaxes to a (3×1) dimerized configuration. However, if we take as an initial point the (3×2) interstitial geometry found in Ref. 16, the relaxed system displayed the (3×2) interstitial configuration with a total energy somewhat lower than that for the (3×1) structure. This is indicative of the stability of the interstitial (3×2) geometry on the (113) Si surface and is in agreement with Ref. 16. We found that the hydrogenated (113) surface has a (3×1) dimerized structure. The atomic geometry of the (113) Si surface found in this work is in agreement with recently published results,[16–18] which describe in detail this structure. The Si(001) surface is characterized by asymmetric (2×1) [bare Si(001) surface] or symmetric (2×1) [hydrogenated Si(001) surface] dimers, in agreement with previous works.[6,19,20]

III. REFLECTANCE ANISOTROPY SPECTRA

Calculated atomic geometries were used as an input for the determination of the optical functions and the RA spectra. For the numerical study of the SIOA we used the DFT-LDA method by taking into account a nonlocality of pseudopotentials in calculations of the optical matrix elements.[21] For the surface optical functions we also include quasiparticle (QP) corrections to DFT-LDA eigenenergies calculated for bulk Si with LDA wave functions. Calculated QP shifts were further reduced by a factor 0.5 to match experimental values of E_1 and E_2 critical point energies as described in Ref. 21. These self-energy corrections differ from a pure scissors-operator-like shift in the optical spectrum because it includes an energy dependence of QP values.[21] In this study the effect of the microscopic local field (LF) is neglected.

In the calculations of optical functions to obtain reliable and good converge results we used up to 32 layers in a slab and 64 special k points in the surface BZ. To simplify a numerical procedure for more complicated surface configurations we used SETBM.[6,22–24] The surface optical functions have been calculated by SETBM using a sp^3s^* tight binding basis, and by parametrization of the intra-atomic matrix elements of the momentum operator.[25] This theoretical model has been used on different covalent as well as ionic semiconductors.[6] We demonstrate below that for silicon SETBM provides reliable results which agree with *ab initio* theory and experimental results.

The imaginary part of the complex dielectric functions $(\epsilon_{2,b})$ of bulk Si as calculated with the SETBM and DFT-LDA methods are shown in Fig. 1 in comparison with experimental data.[26] We denote by arrows the calculated SETBM positions of the E_1 and E_2 peaks in Fig. 1. The real part of the dielectric function $(\epsilon_{1,b})$ of bulk Si has been computed directly by the DFT-LDA method, while the Kramers-Kronig relations were used for the calculation of $\epsilon_{1,b}$ by SETBM.

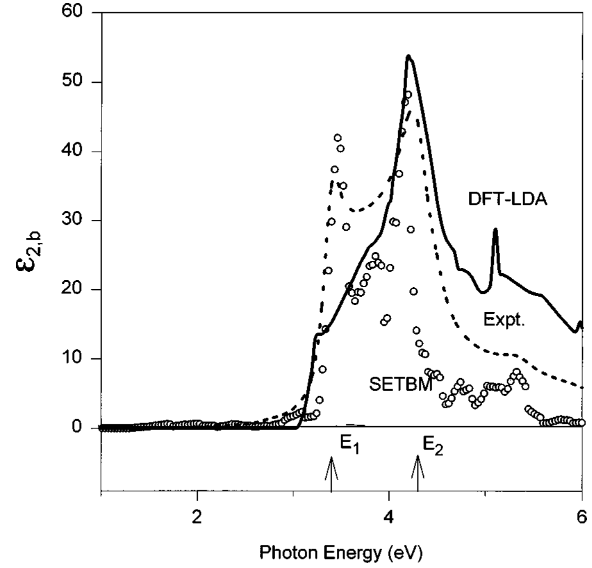

FIG. 1. The imaginary part of dielectric function of bulk Si calculated with *ab initio* DFT-LDA theory (solid line) and by SETBM (dotted line) are shown in comparison with the experimental data (dashed line) of Ref. 26. The arrows denote the calculated SETBM positions of the E_1 and E_2 energies.

It has been stated previously[27] that the E_1 structure cannot be described theoretically within the random phase approximation method by neglecting excitonic effects. Our *ab initio* $\epsilon_{2,b}$ spectrum of Si (see solid line in Fig. 1) shows only a shoulder in the region of the E_1 transitions in agreement with other first-principles studies.[19,21] However, our SETBM results (dotted line in Fig. 1) show a peak in the E_1 region. This is a consequence of the fact that by proper choice of empirical parameters that describe the optical matrix elements one can simulate (at least partially) excitonic effects.[6]

The RA spectra of the silicon surfaces were calculated according to the scheme described in Refs. 27 and 28. The complex anisotropy of the surface reflectance of the normally incident light is given by[6,7]

$$\frac{\Delta\tilde{r}}{\tilde{r}}=\frac{\Delta R}{R}+i\Delta\phi. \tag{1}$$

The expression $\Delta\tilde{r}/\tilde{r}$ can be calculated from the optical constants by[11]

$$\frac{\Delta\tilde{r}}{\tilde{r}}=-\frac{2iEd}{\hbar c}\frac{\epsilon_\alpha-\epsilon_\beta}{\epsilon_b-1}, \tag{2}$$

where E is the photon energy and d is the thickness of the anisotropic overlayer. The quantities ϵ_α and ϵ_β are the components of the surface dielectric tensor along α and β, respectively, and ϵ_b is the complex bulk dielectric function. We choose α and β to be along $[110]$ and $[1\bar{1}0]$, respectively. In order to account for the finite number of $\mathbf{k}$ points in

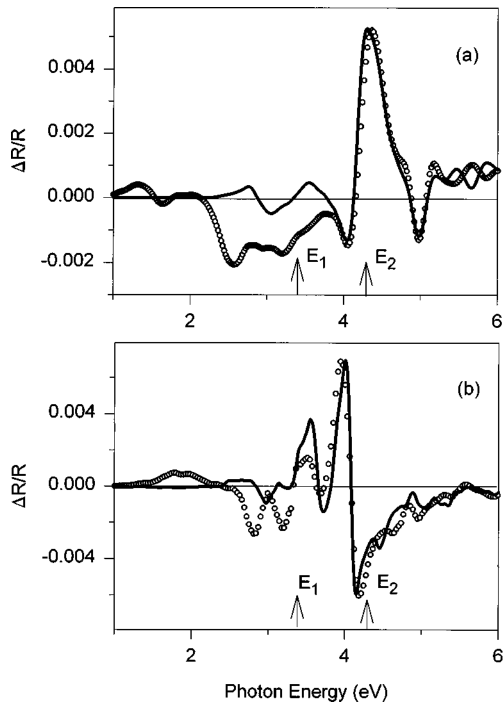

FIG. 2. Calculated RA spectra of clean (dotted line) and hydrogenated (2×1) (001) (solid line) Si surfaces obtained with (a) *ab initio* DFT-LDA theory and (b) SETBM. The arrows denote the calculated positions of the E_1 and E_2 energies of bulk Si.

our calculations we use an energy broadening of 0.1 eV taken into the **k**-point sampling of the irreducible part of the BZ.

In Fig. 2 the RA spectra of clean and hydrogenated Si(001) (2×1) surfaces as calculated both by *ab initio* theory [Fig. 2(a)] and by SETBM [Fig. 2(b)] are presented. The arrows denote the calculated positions of the E_1 and E_2 energies. Our analysis shows that the optical response of the clean (001) (2×1) Si surface in the region 1.3–2.5 eV [see dotted lines in Fig. 2(a) and Fig. 2(b)] is caused by the optical transitions between bonding and antibonding dangling bond states. The dangling bonds are located on asymmetric dimers, in agreement with previous studies.[29] For the RA spectroscopy response around 3.0 eV, the optical transitions between surface and bulk states are responsible.

It is instructive to compare the RA spectra calculated by the SETBM and DFT-LDa methods (see Fig. 2). The results of our semiempirical calculations [Fig. 2(b)] are in good agreement with the *ab initio* predictions [Fig. 2(a)] in the regions of the surface-to-surface and surface-to-bulk optical transitions of the (001) Si surface. The RA spectra obtained by both methods in the region around the E_1 bulk transitions are also in good agreement. This corresponds to the interval 1.5–3.7 eV [see Figs. 2(a) and 2(b)]. There are remarkable discrepancies between the SETBM data and our *ab initio* predictions in the high-energy region. The reason for this is the well-known problems of realistic description of higher conduction bands with a tight binding theory.[22]

The atomic structure of the (113) Si surface is much more complicated than that of the (001) Si surface.[16] The effect of the double steps on the RA spectra of the (113) Si surface can be represented as a (001) surface with vicinal angle of 25.23°. Consequently the (113) Si surface can be considered

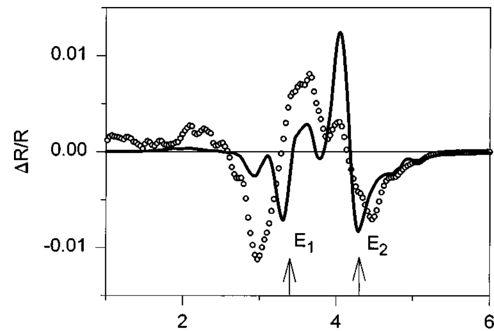

FIG. 3. Calculated RA spectra of bare (3×2) (113) (dotted line) and hydrogenated (3×1) (113):H (solid line) silicon surfaces calculated by SETBM. The arrows denote the positions of the E_1 and E_2 energies of bulk Si.

as a surface effectively composed of high density double height Si (001) steps.[1] For the sake of simplicity we used only SETBM for this surface. The surface optical functions in the region of E_1 and E_2 transitions converge quite slowly with a number of the layers in the slab. We used a 32-layer slab to obtain optical functions for the (113) (3×2) and the (113) (3×1):H surfaces by SETBM. In Fig. 3 the influence of hydrogen adsorption on the calculated RA spectra has been demonstrated. The RA spectra of the bare (113) (3×2) Si surface (see dotted line in Fig. 3) show a strong response in the region around 3.0 eV that disappears after adsorption of hydrogen (cf. solid line in Fig. 3). The RA signal of the bare (113) (3×2) Si surface in the region around 3.0 eV is related to surface-to-bulk transitions.

In Fig. 4 we compare the RA spectra calculated by SETBM for the (001) (dotted line) and the (113) (solid line) Si surfaces covered with hydrogen. The most important difference between these spectra occur in the region of the E_1 transition: the RA response on the (113) surface (solid line in Fig. 4). This clearly indicates that SIOA caused by double steplike atomic geometry is remarkably stronger that SIOA induced by dimerlike surface geometry.

IV. DISCUSSION

Our outcomes obtained by both *ab initio* theory and SETBM on the (001) Si surface show a RA spectroscopy

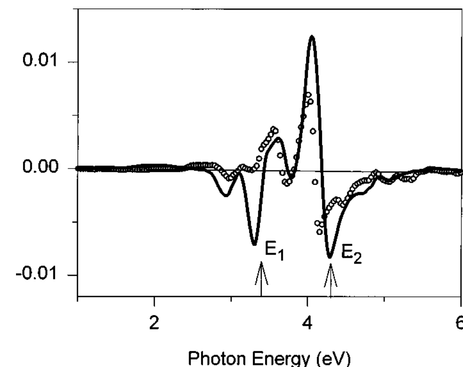

FIG. 4. Calculated RA spectra of the hydrogenated (113) (3×1):H (solid line) and (001) (2×1):H (dotted line) silicon surfaces calculated by SETBM. The arrows denote positions of the E_1 and E_2 energies of bulk Si.

response in the region 1.0–2.2 eV, which is related to surface-to-surface optical transitions between bonding and antibonding surface states (see Fig. 2). These surface states are caused by the dangling bonds located on asymmetrical dimer atoms. This part of the RA spectrum agrees well with the previous results of an SETBM study of RA spectroscopy on Si(001).[29] Surface-to-bulk transitions are responsible for a strong negative peak in the region from 2.6 to 3.1 eV [Figs. 2(a) and 2(b)]. Similar RA spectra of the (001) Si surface have been reported recently in Ref. 19, where the DFT-LDA method with semiempirical QP corrections has been used. On a clean (113) Si surface the relevant RA spectroscopy response is much stronger and located close to 3.0 eV (see dotted line in Fig. 3). Thus our results can account for the experimental observation that the intensity of the RA spectroscopy signal in the region of 3 eV is much stronger on the (113) surface compared with (001) Si surfaces.[1,2,11] To illustrate this point we display in Fig. 6 the RA spectra from vicinal Si surfaces taken from Ref. 1.

On clean (113) Si surface two broad peaks located at 1.0 and 2.0 eV related to surface-to-surface type optical transitions and the strong negative peak at 3.0 eV are caused by surface-to-bulk type of transition (see dotted line in Fig. 3). One can conclude that the calculated enhancement of RA spectroscopy response near 3.0 eV is caused by a dangling bond configuration related to the double steplike atomic geometry. Measured RA spectra of clean reconstructed Si vicinal (001) surfaces showed both a broad structure near 3.0 eV and a second future near 4.3 eV that occurred near the E_2 peak of bulk Si.[1,2,4,11] This is consistent with our results presented in Fig. 2.

The value of the calculated SIOA related to the bulk electron states in the region of E_2 is quite strong on both the (001) and the (113) Si surfaces (see Figs. 2 and 3). However, the predicted RA spectroscopy response in the region of the E_1 transition on the (001) surface is remarkably lower than that on the (113) surface (see Fig. 4). As mentioned above, the surface atomic configuration of the (113) surface is remarkably different that the (001) (2×1) surface. On the hydrogen passivated (113) surface a RA spectroscopy peak near 3.3 eV is predicted (see Fig. 3). This signal corresponds to the E_1 transition in bulk Si. It is very weak on the (001) surface, as shown in Fig. 4 by the dotted line. The reason for this effect is an enhancement of SIOA on the (113) surface caused by the double steplike atomic configuration. Our results show that SIOA induced by the double steplike atomic configuration is much stronger than SIOA caused by dimerized (2×1) geometry.

Let us consider further the line shape of the predicted RA spectrum on the hydrogenated (113) Si surface. One of the main results of Refs. 1, 2, and 11 was that the line shape of the RA spectra from the hydrogenated vicinal (001) and (113) surfaces is like the first derivative of the bulk dielectric function. We will demonstrate below that our calculated RA spectroscopy signal can account for this observation. Since RA spectroscopy is a form of ''external'' modulation spectroscopy the relative changes in the reflectivity can be expressed in terms of the changes in the real ($\Delta\epsilon_{1,b}$)and imaginary ($\Delta\epsilon_{2,b}$) components of ϵ_b as[30]

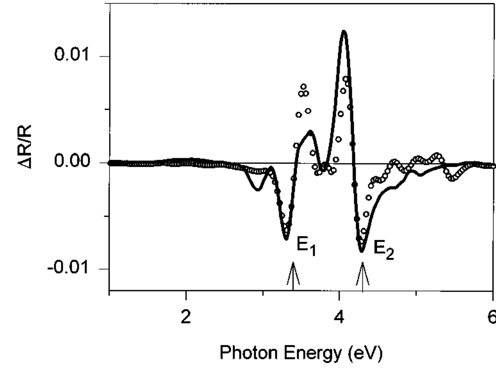

FIG. 5. Calculated RA spectrum for the hydrogenated (3×1) (113):H silicon surface (solid line) in comparison with the $\Delta R/R$ spectrum (dotted line) obtained from Eq. (4) with $\Theta(E_1)=-75°$ and $\Theta(E_2)=30°$, where ϵ_b of bulk Si was calculated by SETBM. The arrows denote the calculated SETBM positions of the E_1 and E_2 energies of bulk Si.

$$\frac{\Delta R}{R}=a[\epsilon_{1,b}(E),\epsilon_{2,b}(E)]\Delta\epsilon_{1,b}(E)+b[\epsilon_{1,b}(E),\epsilon_{2,b}(E)]\Delta\epsilon_{2,b}(E), \quad (3)$$

where a and b are the Seraphin coefficients.[30] Equation (3) can be rewritten as

$$\frac{\Delta R}{R}=A\ \mathrm{Re}[e^{i\Theta(E)}\Delta\epsilon_b(E)], \quad (4)$$

where A is an amplitude and $\Theta(E)$ ($\tan\Theta=a/b$) is a phase factor that describes the admixture between $\Delta\epsilon_{1,b}$ and $\Delta\epsilon_{2,b}$. In our case we take $\Delta\epsilon_b=(d\epsilon_b/dE)\Delta E$, i.e., a first-derivative spectroscopy.

The solid line in Fig. 5 shows the RA spectrum of the hydrogenated (113) Si calculated using Eq. (2). The dotted line displays the RA spectroscopy response determined using Eq. (4), where we have obtained $d\epsilon_b/dE$ from ϵ_b calculated by SETBM (see Fig. 1). In order to get good agreement between the two curves we have taken for Eq. (4) the values $\Theta(E_1)=-75°$ and $\Theta(E_2)=30°$ for the E_1 and E_2 features, respectively. These values of Θ can be verified by determining a and b from the optical constants obtained either from (i) our theoretical SETBM calculation (dotted line in Fig. 1) or (ii) the experimental data (dashed line in Fig. 1). We find $\Theta(E_1)=-82°$, $\Theta(E_2)=28°$, and $\Theta(E_1)=-71°$, $\Theta(E_2)=45°$ in the former and latter case, respectively, in good agreement with the results shown in Fig. 5.

Our results demonstrate that the calculated RA spectrum of the hydrogenated (113) surface indeed corresponds to the first derivative of the bulk dielectric function of silicon. These are consistent with experimental data (see Fig. 6) obtained on the hydrogen passivated (113) Si surface,[1,2,4,11] where a strong derivativelike RA spectroscopy signal has been measured in the E_1 and E_2 transition regions.

While our theoretical results can account for the general properties of the experimental spectra of Fig. 6, i.e., increase of signal with vicinal angle and first-derivative-like nature of the spectra, they cannot duplicate the exact details of the experiment. This is due to several causes. For example, we have ''simulated'' the excitonic nature of the E_1 transition in

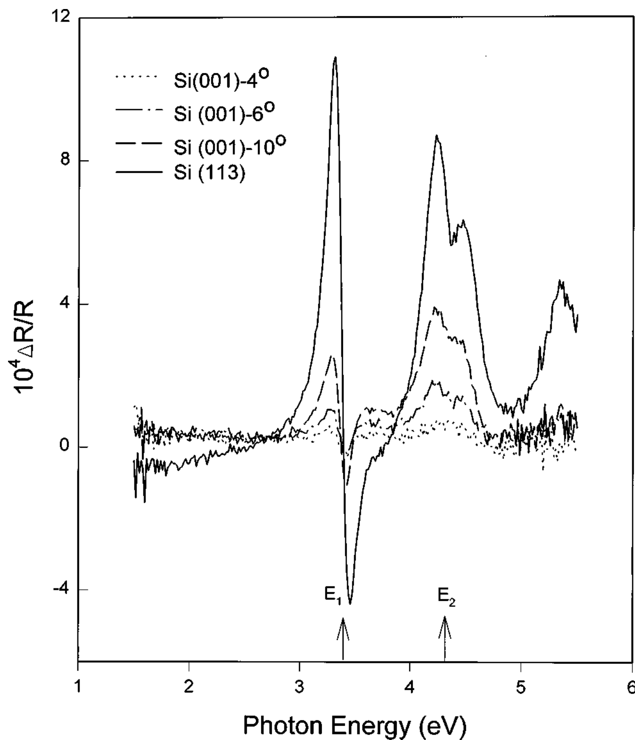

FIG. 6. Experimental RA spectra for vicinal Si surfaces (from Ref. 1). The arrows denote positions of the E_1 and E_2 energies of bulk Si. Reprinted from Appl. Surf. Sci. **107**, 35 (1996) with permission from Elsevier Science.

the SETBM calculation by the procedure mentioned above. However, the E_1 peak in the experimental optical constants (see Fig. 1) has an excitonic Lorentzian line shape while for our theoretical one-electron SETBM calculation the line shape is that of a two-dimensional critical point. The derivative of the former is narrower and more intense in relation to the latter.[30] Also, as pointed out above, the SETBM method does not account properly for the conduction bands that contribute to the E_2 feature.

The phase of the calculated RA spectra in Fig. 5 are almost opposite to that of the experimental data of Fig. 6. According to the Koster-Slater model[30] excitonic effects also can significantly alter the values of the phase angle Θ. These effects are much stronger at E_1 in relation to E_2, because of the excitonic nature of the former. Therefore, this effect also demonstrates that in order to get better agreement between experiment and theory the electron-hole interaction should be included explicitly.

It is instructive to analyze further the optical anisotropy of Si surfaces. The atomic configurations of the (001) and (113) Si surfaces used in this work for the calculation of the RA spectra do not show any new details as compared with previously published results.[6,16–18,20,29] Strong distortions of the atomic geometry of the surface atoms cause dramatic changes in the surface electron energy structure and consequently the optical functions related to electronic transitions, which involve either surface states or electronic states related to the back bonds of the surface atoms. This point has already been made in Refs. 6 and 31. The distortion of the atomic bonds of more deeply lying atomic layers is much less pronounced and hence they cause relatively small changes of the electron energy structure. These changes are well oriented on the surface due to dimer and steplike geometries. As has been studied in detail in Ref. 6 the physical nature of the optical anisotropy of Si surfaces in the region of the E_1 and E_2 transitions is surface induced distortions of bulklike atomic bonds of deep-lying near-the-surface atomic layers. In addition to the previous studies our results show that the steplike distortions provide much stronger SIOA than dimers.

V. SUMMARY

We have reported the results of a theoretical study of the SIOA of the (001) and (113) Si surfaces by the use of first-principles density functional theory and the semiempirical tight binding model. The optical response of clean (001) and (113) surfaces obtained in the region around 3.0 eV originates from surface-to-bulk transitions. A strong SIOA response has determined in the region of the E_1 and E_2 bulk critical points. The line shape of this response corresponds to the first derivative of the dielectric function of bulk Si. The derivativelike optical features in the vicinity of E_1 are much stronger on the (113) surface in relation to the (001) case due to distortions resulting from the double-steplike atomic geometry. The obtained results account for a number of experimental observations.

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[1] L. Mantese, U. Rossow, and D. E. Aspnes, Appl. Surf. Sci. **107**, 35 (1996).

[2] U. Rossow, L. Mantese, and D. E. Aspnes, *Proceedings of the 23rd International Conference on the Physics of Semiconductors, Berlin, 1996*, edited by M. Scheffler and R. Zimmermann (World Scientific, Singapore, 1996), p. 831.

[3] G. P. M. Poppe, H. Wormeester, A. Molenbroek, C. M. J. Wijers, and A. Van Silfhout, Phys. Rev. B **43**, 12 122 (1991).

[4] S. G. Jaloviar, J. L. Lin, and M. G. Lagally, Bull. Am. Phys. Soc. **42**, 618 (1997).

[5] F. H. Pollak and H. Shen, Mater. Sci. Eng., R. **10**, 275 (1993).

[6] R. Del Sole, in *Photonic Probes of Surfaces*, edited by P. Halevi (Elsevier, Amsterdam, 1995), p. 131.

[7] T. Nakayama, Phys. Status Solidi B **202**, 741 (1997).

[8] See, for example, T. Holden, F. H. Pollak, J. L. Freeouf, D. McInturff, J. L. Gray, M. Lundstrom, and J. M. Woodall, Appl. Phys. Lett. **70**, 1107 (1997), and references therein.

[9] L. F. Lastras-Martinez and A. Lastras-Martinez, Phys. Rev. B **54**, 10 726 (1996).

[10] Z. Yang, G. K. Wong, I. K. Sou, and Y. H. Yeung, Appl. Phys. Lett. **66**, 2235 (1995).
[11] U. Rossow, L. Mantese, and D. E. Aspnes, J. Vac. Sci. Technol. B **14**, 3070 (1996).
[12] L. Kleinman and D. M. Bylander, Phys. Rev. Lett. **48**, 1425 (1982).
[13] R. Stumpf and M. Scheffler, Comput. Phys. Commun. **79**, 447 (1994).
[14] D. M. Ceperley and B. I. Alder, Phys. Rev. Lett. **45**, 566 (1980).
[15] P. Perdew and A. Zunger, Phys. Rev. B **23**, 5048 (1981).
[16] J. Dabrowski, H.-J. Mussig, and G. Wolff, Phys. Rev. Lett. **73**, 1660 (1994).
[17] J. Schreiner, K. Jacobi, and W. Selke, Phys. Rev. B **49**, 2706 (1994).
[18] S. van Dijken, H. W. Zandvleit, and B. Poelsema, Phys. Rev. B **55**, 7864 (1997).
[19] Y.-C. Chang, G. Li, and L. Li, Bull. Am. Phys. Soc. **42**, 618 (1997).
[20] P. Kruger and J. Pollmann, Phys. Rev. B **47**, 1898 (1993).
[21] V. I. Gavrilenko and F. Bechstedt, Phys. Rev. B **55**, 4343 (1997).
[22] W. A. Harrison, *Electronic Structure and Properties of Solids* (W. H. Freeman, San Francisco, 1980).
[23] V. I. Gavrilenko, P. Vogl, and F. Koch, in *Microcrystalline Semiconductors: Materials Science and Devices*, edited by P. M. Fauchet *et al.*, MRS Symp. Proc. No. 283 (Materials Research Society, Pittsburgh, 1993), p. 431.
[24] V. I. Gavrilenko, Appl. Phys. Lett. **67**, 16 (1995).
[25] R. Del Sole, Solid State Commun. **37**, 537 (1981).
[26] D. E. Aspnes and A. A. Studna, Phys. Rev. B **27**, 985 (1983).
[27] R. Del Sole and R. Girlanda, Phys. Rev. B **54**, 14 376 (1996).
[28] F. Manghi, R. Del Sole, A. Selloni, and E. Molinari, Phys. Rev. B **41**, 9935 (1990).
[29] A. I. Skrebtii and R. Del Sole, Phys. Rev. Lett. **70**, 2645 (1993).
[30] D. E. Aspnes, in *Handbook on Semiconductors*, Vol. 2, edited by M. Balkanski (North-Holland, New York, 1980), p. 109; M. Cardona, *Modulation Spectroscopy* (Academic, New York, 1969).
[31] V. I. Gavrilenko and F. Koch, J. Appl. Phys. **77**, 3288 (1995).