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LETTER TO THE EDITOR

In-plane optical anisotropy in asymmetric $Si_{1-x}Ge_x/Si/Si_{1-y}Ge_y$ superlattices

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Abstract
A trilayer asymmetric superlattice, $Si/Si_{1-x}Ge_x/Si_{1-y}Ge_y$, is proposed, in which the broken inversion symmetry makes the microstructure optically biaxial; in particular, inequivalent interfaces in this heterostructure may cause a polarization ratio as large as about 2.5% in the absence of an external field. The electronic structure and absorption spectra for two types of trilayer superlattice with different parameters are calculated by use of the tight-binding model; the findings indicate the importance of the carrier confinement for the anisotropy value. The effect of external electric field on the optical anisotropy for such structures has also been discussed, and a Pockels coefficient of 10^{-9} cm V^{-1} estimated.

Silicon is the most important material for information technology. Owing to very advanced and sophisticated LSI technology, the use of Si-based structures in all-optical or electro-optical device applications has naturally attracted a lot of research interest, though bulk Si is not considered a promising candidate for light-emitting materials because of its indirect-band-gap nature, nor as a nonlinear-optical material because of the O_h point-group symmetry.

The development of heterostructures paves the way for using silicon in light emission applications. The quantum confinement effect in silicon-based structures breaks the quasi-momenta conservation law and hybridizes many bulk band states; this led to the observation of photoluminescence in Si/Si_xGe_{1-x} strained quantum wells and superlattices, which has been subsequently intensively studied [1, 2]. On the other hand, since they have inversion symmetry, bulk silicon and Si superlattices have found little application in second-order nonlinear optics.

Inversion asymmetry governs a variety of properties in semiconductors, such as the lifted twofold degeneracy of the band dispersion, the spin-orientation phenomena, and the second-order optical nonlinearities including optical rectification and field-induced birefringence (the Pockels effect), which is important for modulation, switching in optoelectronic circuits, and phase matching in nonlinear optics [3]. Recently, giant quantum-confined Pockels effects have been experimentally detected in a variety of quantum wells including the type-I quantum wells where the well and barrier share a common atom [4], the type-I quantum wells with no common atom [5], and type-II quantum wells [6], which has given rise to a lot of research

interest in this topic [7–11]. However, since all such research is concentrated on III–V or II–VI group semiconductor systems, such as the GaAs/AlAs, GaAs/InP, and ZnSe/BeTe systems, a question has arisen: can the silicon-based structure be useful in birefringence and linear electro-optics?

Usually, inversion asymmetry originates from the bulk intrinsic nature, an applied external potential, and the inequivalent interfaces in heterostructures. For Si-based systems, the non-zero second-order nonlinearity comes only from the inequivalent interfaces. The [001]-oriented Si/GeSi quantum wells and superlattices are of point-group symmetry D_{2d}, which is uniaxially isotropic for normal incidence. Like for quantum wells with no common atom, if a special Si-based structure with the point-group symmetry C_{2v} can be created by introducing inequivalent interfaces, the silicon-based superlattice may be biaxial, and its second-order nonlinear susceptibility could no longer be equal to zero. Thus, combined with well-developed silicon technology, it is expected to have potential application in future optoelectronic devices.

In this letter, we intend to propose a silicon-based asymmetric superlattice, namely $Si/Si_{1-x}Ge_x/Si_{1-y}Ge_y$ ($x = 0.25$, $y = 0.5$), in which lack of inversion and rotoinversion centres in the microstructure leads to an in-plane anisotropy in the absorption spectra. We shall evaluate the absorption spectra on the basis of the band structure by using the empirical tight-binding method. In addition to the anisotropic optical spectra in the absence of applied field, we will also estimate the anisotropic optical response to an external DC field and the magnitude of the Pockels coefficient for this novel structure.

The conventional envelope function theory, which is successful in interpreting a lot of optical and electric properties in quantum well systems, has failed to explain the in-plane optical anisotropy in quantum wells with inequivalent interfaces, because the envelope function takes no account of the real bond orientation and structure in the vicinity of superlattice interfaces [12]. In view of the fact that tight-binding theory gives a full description for the local symmetry of a real superlattice [13], yet is still simple, in this letter we shall adopt the empirical tight-binding model to calculate the electronic structure and optical absorption spectra of the $Si/Si_{1-x}Ge_x/Si_{1-y}Ge_y$ superlattice. Here we assume that the trilayer structure repeats itself to form a superlattice on a Si substrate, with the z-axis as the growth direction. The superlattice state associated with band index n and wavevector $\vec{k}$ can be expressed as

$$|n, \vec{k}\rangle = \sum_{\alpha,I} C_{n,\alpha,I} \sum_{\vec{R}} \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{R}} |\alpha, I, \vec{R}\rangle \tag{1}$$

where α, I, and $\vec{R}$ denote the orbital type, the basis atom, and the atom position in a superlattice cell, respectively, and the $C_{n,\alpha,I}$ are the expansion coefficients of the Bloch sum associated with α and I. The sp^3s^* atomic orbitals, with the nearest-neighbour coupling model [14] and spin–orbit coupling [15], are used in the present calculation. Thus, for each atom there are ten orbitals with the spin index included.

The bond lengths and tight-binding parameters for bulk Si and Ge are taken from reference [14], while those for SiGe alloys are obtained by interpolating the values for bulk Si and Ge [16]. The interatomic matrix elements connecting the Si atom and GeSi alloy atom across the interfaces are taken from the arithmetic mean values of their corresponding bulk parameters. The strain effect is accounted for in a rather simple way [17]—namely, the interatomic matrix elements $H_{\alpha,\beta}$ for the strained structure are deduced from the strain-free ones, $H^0_{\alpha,\beta}$, through

$$H_{\alpha,\beta} = H^0_{\alpha,\beta}(d_0/d)^2$$

where d and d_0 are the bond lengths with and without strain, respectively. The valence band offset for $Si_{1-x}Ge_x$ grown on a Si substrate is taken as $740x$ meV [18]. Following the

approximation used in reference [19], the matrix elements for the interband optical transition can readily be worked out as

$$\vec{p}_{c,v}(\vec{k}) = \frac{m_0}{\hbar} \sum_{\alpha,\beta,I,J} C^*_{c,\alpha,I}(\vec{k}) C_{v,\beta,J}(\vec{k}) \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \vec{R} H_{\alpha,\beta,I,J}(\vec{R}) \tag{2}$$

where $H_{\alpha,\beta,I,J}$ comes from the tight-binding parameters, and $C_{c,\alpha,I}(\vec{k})$ and $C_{v,\beta,J}$ are the envelope functions of the conduction and valence subbands respectively. The optical absorption is then written as

$$\alpha_{\hat{\epsilon}} = \frac{A}{\omega} \sum_{c,v,\vec{k}} |\hat{\epsilon} \cdot \vec{p}_{c,v}(\vec{k})|^2 \delta\{\omega - [E_c(\vec{k}) - E_v(\vec{k})]\} \tag{3}$$

where A is a constant and $\hat{\epsilon}$ is a unit vector denoting the polarization direction of the incident light with energy ω. The summation runs over the whole Brillouin zone. A Lorentzian $\gamma/(\gamma^2 + \omega^2)$ is used to approximate the delta function $\delta(\omega)$. In our calculation, 72 points in one quarter of the Brillouin zone are used, and the parameter γ is equal to 20 meV.

When the incidence is along [001], the difference in absorption spectra between [110] and $[\bar{1}10]$ polarization is expected not to be zero because of the C_{2v} symmetry of the system. We scale this in-plane anisotropy by defining the polarization ratio (PR) as

$$\mathrm{PR} = \frac{\alpha_{[110]} - \alpha_{[\bar{1}10]}}{\alpha_{[110]} + \alpha_{[\bar{1}10]}}. \tag{4}$$

When a DC electric field is applied to the structure along the superlattice growth direction, a term, $eF\vec{z}$, is added to the Hamiltonian. Suppose that the barriers are so thick that we can safely ignore the coupling of two neighbouring quantum wells by the field. Then the effect of the applied field on the system Hamiltonian can be approximated as an added diagonal term only [7, 20, 21]; the result reads

$$\begin{aligned} \langle \alpha, I, \vec{R} | eF\vec{z} | \beta, J, \vec{R}' \rangle &\approx \langle \alpha, I, \vec{R} | eF\vec{z} | \alpha, I, \vec{R} \rangle \delta_{\alpha,\beta} \delta_{I,J} \delta_{\vec{R},\vec{R}'} \\ &= [\langle \alpha, I, \vec{R} | eF(\vec{z} - Z) | \alpha, I, \vec{R} \rangle + eFZ] \delta_{\alpha,\beta} \delta_{I,J} \delta_{\vec{R},\vec{R}'} \\ &= [eFZ] \delta_{\alpha,\beta} \delta_{I,J} \delta_{\vec{R},\vec{R}'} \end{aligned} \tag{5}$$

in which Z is the [001] component of the atomic position vector. The first term in the second line of the formula above vanishes for symmetry reasons.

The band structures of two trilayer superlattices with two different layer thicknesses, $(Si)_{80}/(Si_{0.75}Ge_{0.25})_{20}/(Si_{0.5}Ge_{0.5})_8$ (SL1) and $(Si)_{32}/(Si_{0.75}Ge_{0.25})_8/(Si_{0.5}Ge_{0.5})_{72}$ (SL2), have been calculated. Figure 1 shows the dispersion relations of the two structures in the absence of the field. For several of the lowest subbands, the Si layers are the wells for electrons and the $Si_{0.5}Ge_{0.5}$ layers play the role of the wells for holes. Thus the type-II superlattice has lower transitions to some extent; the asymmetry is thus enhanced further. For higher subbands, a zone-folding effect is evident, as shown in figure 1. The envelope functions of the first valence subband (VB1) at the Brillouin zone centre for the two superlattices are presented in figure 2. Clearly, in both superlattices the holes are mainly confined to the $Si_{0.5}Ge_{0.5}$ layers. The well width plays a very important role in determining the distribution of the confined holes. For SL1 with thin $Si_{0.5}Ge_{0.5}$ wells, the higher quantization energy causes a significant penetration into the barrier region for the envelope function of VB1, which is highly asymmetric because of the significant difference between the barrier heights in the $Si_{0.75}Ge_{0.25}$ and in Si layers. The envelope function of VB1 in SL2 has a small amplitude at the interfaces and is nearly symmetric with respect to the well centre because of the lower confined energy in the thicker wells.

The absorption spectra along the [110] and $[\bar{1}10]$ directions are calculated, with over 100 valence subbands and 200 conduction subbands involved, and the corresponding polarization

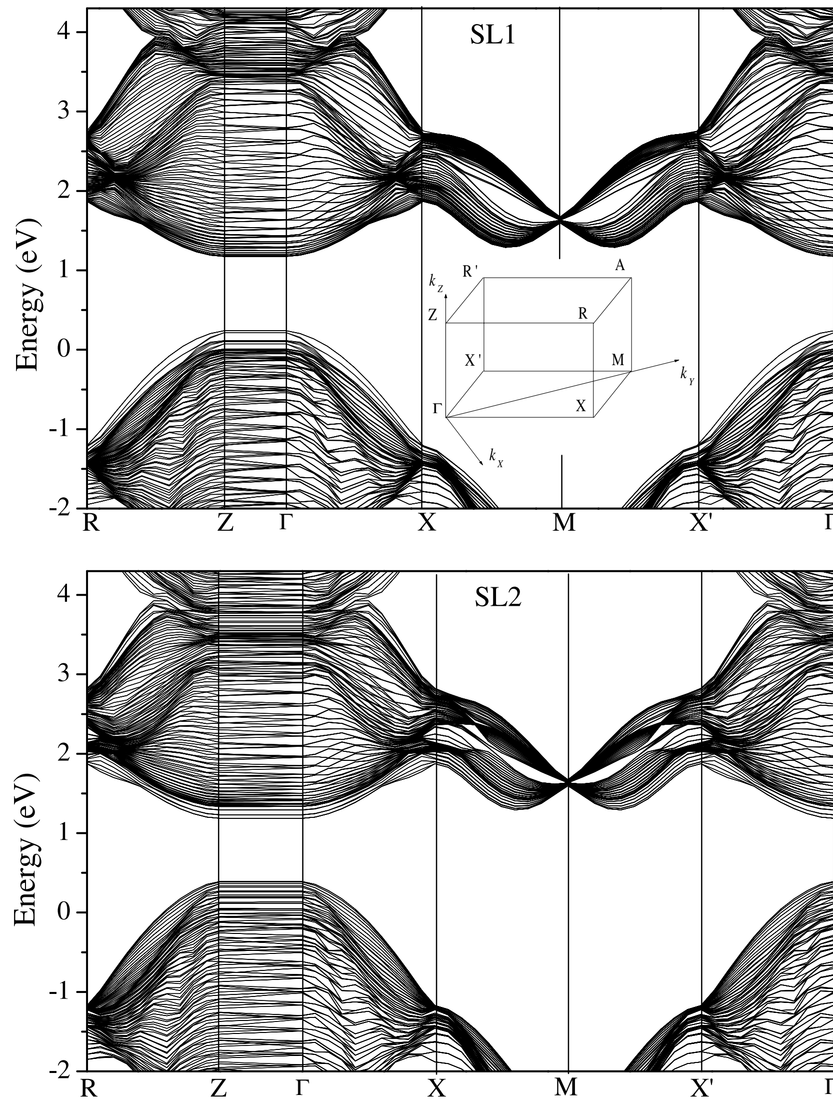

Figure 1. Subband dispersion relations for the $Si_{1-x}Ge_x/Si/Si_{1-y}Ge_y$ superlattices. The inset displays the irreducible part of the Brillouin zone.

ratios for the two structures are displayed in figure 3. As shown in the figure, the polarization ratio in SL1 is significant over the incident light energy range from 2.6 eV to 3.0 eV, below the direct absorption edge. The peak value of PR is as large as about 2.5%, which is remarkable in view of the vanishing value of PR in bulk silicon or germanium. On the other hand, PR for SL2 is a little less than 1%. This value of PR stems from the asymmetry of the structure and in particular from the inequivalent interface regions, because of the type-II confinement character. The difference between the values of PR for the two samples comes from the quantum confinement of carriers as mentioned above, though only the effect of confinement of VB1 on PR has been discussed. For the sake of comparison, we have also analysed the respective contribution to PR from several other valence subbands, verifying that

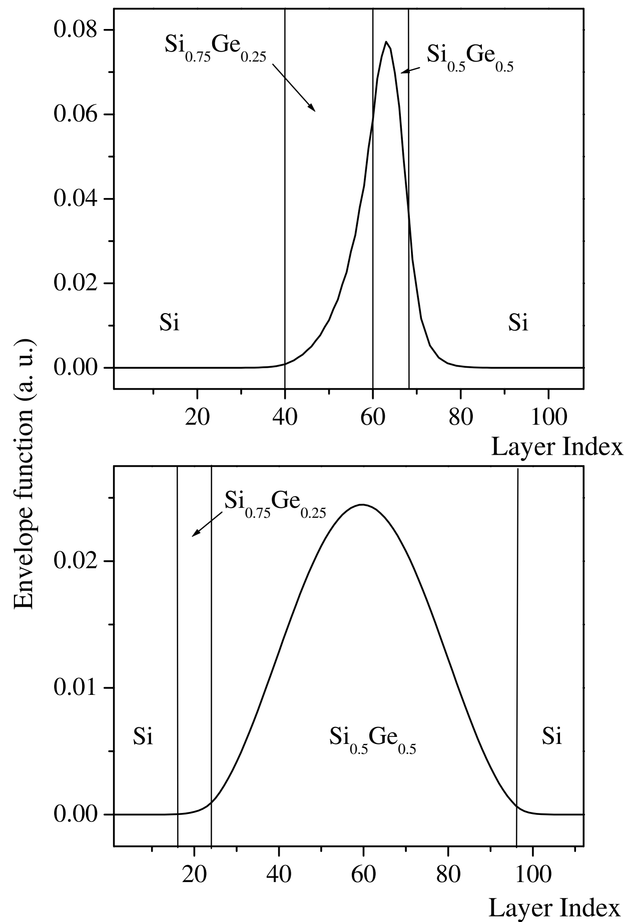

Figure 2. Envelope functions for the first valence subband at the Γ point. Top: SL1; bottom: SL2.

the contribution exclusively comes from VB1, as the effect of confinement on VB1 is the strongest. We thus believe that the in-plane anisotropy in the proposed structures derives from the interface asymmetry, and the magnitude of the anisotropy is sensitive to the electronic structure of the systems.

When a DC electric field is applied along the [001] direction, the external potential will affect the carrier distribution; consequently the linear electro-optical effect is induced. Together with the effects due to the inequivalent interfaces and the quantum confinement of carriers, the applied field affects the in-plane anisotropy in the proposed structures in a subtle way.

The external DC field will make the subband edge shift and the carrier distribution polarize. Being of opposite charge, electrons and holes are driven by the electric field in opposite directions. According to perturbation theory, this effect is proportional to the well thickness. As shown in figure 4, the variation of the hole distribution of VB1 caused by the field is small in the thin well (SL1) but significant in the thick well (SL2). Thus the asymmetry of the VB1 envelope function as well as PR for SL1 remain almost unchanged versus the applied field, while those for SL2 are changed obviously by a moderate field. The more (less) asymmetric redistribution of the carrier induced by the field will favour (disfavour) optical anisotropy.

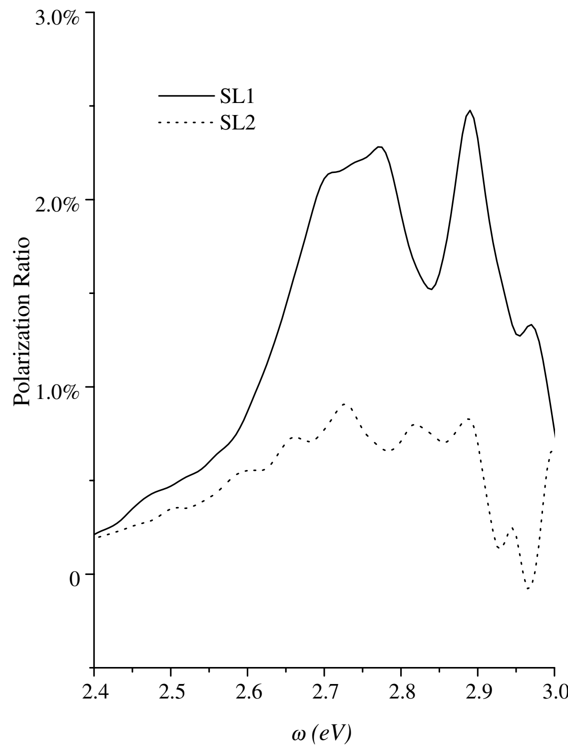

Figure 3. Calculated polarization ratio spectra of SL1 and SL2 under incident [110] and [$\bar{1}$10] polarization.

Because the relative variation of PR versus the external field is small, the Pockels coefficient for the proposed structures, which relates the optical anisotropy response to the external field, is expected to be small compared to that for III–V superlattices. The polarization ratios for several DC-field strengths in SL1 and SL2 are calculated. The results are: PR(0) $= 2.47\%$, PR(25 kV cm^{-1}) $= 2.50\%$, and PR(50 kV cm^{-1}) $= 2.54\%$ for SL1; while PR(0) $= 0.823\%$, PR(25 kV cm^{-1}) $= 0.837\%$, and PR(50 kV cm^{-1}) $= 0.855\%$ for SL2. It has been found that the difference between the absorption spectra along [100] and [010] equals zero for any electric field, indicating that [110] and [$\bar{1}$10] are two principal directions of the dielectric tensor.

We now estimate the Pockels coefficients for these structures. By using the Kramers–Kronig relation, we can transform the absorption coefficient to the refractive index along two principal directions—[110] and [$\bar{1}$10]—of polarization in the presence of the field, $n_{[110]}$ and $n_{[\bar{1}10]}$, and then obtain the Pockels coefficients r_{13} and r_{63} through

$$n_{[110]} = n_1 - \frac{1}{2}n_1^3(r_{13} + r_{63})F \tag{6}$$

$$n_{[\bar{1}10]} = n_2 - \frac{1}{2}n_2^3(r_{13} - r_{63})F \tag{7}$$

where n_1 and n_2 are the refractive indexes for [110] and [$\bar{1}$10] polarization in the absence of the field, respectively.

The Pockels coefficients r_{13} and r_{63} are shown in figure 5 as functions of photon energy. Due to the strong absorption near or above the direct absorption edge, the Pockels coefficient is

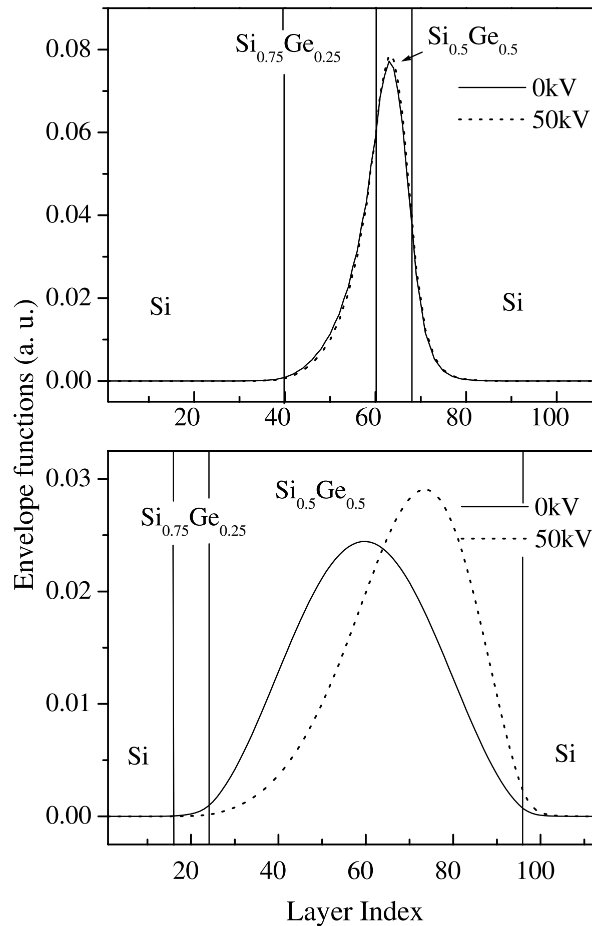

Figure 4. The envelope function of the first valence subband at the Γ point in the absence of electric field (solid line) and in the presence of a DC field of 50 kV cm^{-1} (dashed line). Top panel: SL1; bottom panel: SL2.

well defined only in a much lower energy range. For photon energy $\omega = 1$ eV, the calculated coefficient r_{13} is about 50×10^{-10} cm V^{-1} for SL1 and 8×10^{-10} cm V^{-1} for SL2, while r_{63} is 0.5×10^{-10} cm V^{-1} for SL1 and 1×10^{-10} cm V^{-1} for SL2. r_{63} scales the antisymmetric part of the anisotropy to the electric field. In our calculation, r_{63} is much smaller than r_{13} for both structures.

A novel Si/Si$_{1-x}$Ge$_x$/Si$_{1-y}$Ge$_y$ superlattice has been proposed. The reduced C$_{2v}$ symmetry of the proposed structures leads to a significant optical anisotropy without an electric field. By using the empirical tight-binding model, we have calculated the subband structure and optical anisotropy of two Si/Si$_{1-x}$Ge$_x$/Si$_{1-y}$Ge$_y$ superlattices with different thicknesses with and without an external electric field. The inequivalent interfaces in this system, the carrier-density distribution determined by the quantum confinement, and the external field determine the optical anisotropy in the trilayer Si/SiGe systems. Although the Pockels coefficient for our Si/Si$_{1-x}$Ge$_x$/Si$_{1-y}$Ge$_y$ structures is smaller than that for III–V group superlattices, it may be one order of magnitude larger than that for bulk GaAs even for our non-optimum configuration, which might have some application potential for the future.

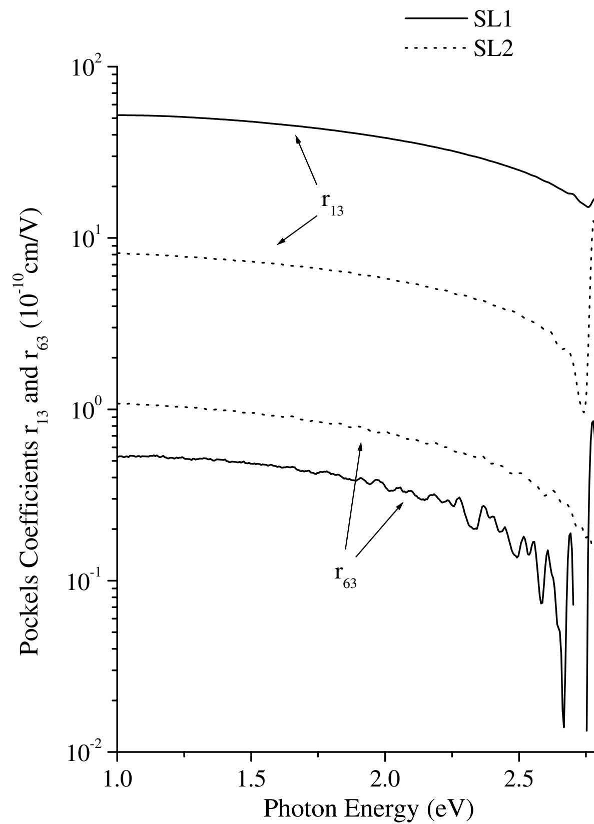

Figure 5. Calculated Pockels coefficients r_{13} and r_{63} as functions of photon energy for SL1 and SL2.

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References

[1] Sturm J C, Manoharan H, Lenchyshyn L C, Thewalt M L W, Rowell N L, Noel J P and Houghton D C 1991 *Phys. Rev. Lett.* **66** 1362
[2] Menczigar U, Abstreiter G, Olajos J, Grimmeiss H, Kibbel H, Presting H and Kasper E 1993 *Phys. Rev.* B **47** 4099
[3] Boyd R W 1992 *Nonlinear Optics* (New York: Academic)
[4] Kwok S H, Grahn H T, Ploog K and Merlin R 1992 *Phys. Rev. Lett.* **69** 973
[5] Krebs O, Rondi D, Gentner J L, Goldstein L and Voisin P 1998 *Phys. Rev. Lett.* **80** 5770
[6] Platonov A V, Kochereshko V P, Ivchenko E L and Mikhailov G V 1999 *Phys. Rev. Lett.* **83** 3546
[7] Zhu B F and Chang Y C 1994 *Phys. Rev.* B **50** 11932
[8] Ivchenko E L, Kaminski A Yu and Rössler U 1996 *Phys. Rev.* B **54** 5852
[9] Khurgin J B and Voisin P 1998 *Phys. Rev. Lett.* **81** 3777
[10] Magri R and Ossicini S 1998 *Phys. Rev.* B **58** R1742
[11] Foreman B A 2000 *Phys. Rev. Lett.* **84** 2505
[12] Krebs O, Voisin P, Rondi D, Gentner J L, Goldstein L and Harmand J C 1999 *J. Physique* IV **9** 37
[13] Schulman J N and Chang Y C 1985 *Phys. Rev.* B **31** 2056
Schulman J N and Chang Y C 1985 *Phys. Rev.* B **31** 2069
[14] Vogl P, Hjalmarson H P and Dow J D 1983 *J. Phys. Chem. Solids* **44** 365

[15] Chadi D J 1977 *Phys. Rev.* B **16** 790
[16] Newman K E and Dow J D 1984 *Phys. Rev.* B **30** 1929
[17] Tserbak C, Polatoglou H M and Theodorou G 1993 *Phys. Rev.* B **47** 7104
[18] Van de Walle C G and Martin R M 1985 *J. Vac. Sci. Technol.* B **3** 1256
[19] Lew Yan Voon L C and Ram-Mohan L R 1993 *Phys. Rev. B* **47** 15 500
[20] Xia J B and Huang K 1988 *Acta Phys. Sinica* **37** 1
[21] Zhu B F 1988 *Phys. Rev.* B **38** 13 316