Theoretical Investigation of Differential Photoreflectance Spectra From Planar-Doped Layers in Semiconductors

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We report on the results of a theoretical investigation of the differential photoreflectance (DPR) spectra. from planar-doped structures. The DPR spectra are simulated by means of a model recently proposed by us, which is based on the common three-dimensional two-particles Franz-Keldysh effect, and takes into account spatial variations of electric field and effective band gap within thc δ-region. The model is applied to a Si δ-layer in GaAs, to a 6-doped structure containing two isolated Si δ-layers, as well as to the interface between undoped and Si heavily-doped degenerated GaAs. The intensity of the DPR signal with the distance between tlie planar-doped layers in the double O-doped structure is examined. A good qualitative agreement between the theoretical results and recent experimental data confirms the validity of tlie present approach.

It has already been demonstrated that photoreflectance (PR) is a powerful spectroscopic technique to investigate the electronic properties of semiconductor heterostructures such as superlattices, quantum-wells and planar (or h-) doped structures[1-7]. The modulation mechanisms and line shapes observed in PR measurements on isolated quantum-wells are reasonably well understood. For these systems, PR signals are due to tlie Starli shifts of sublevels, which result in PR line shapes of first derivative type[1,2]. The Franz-Keldysh (FK) effect becomes important for superlattices with enough wide minibands. FK third derivative like spectra are expected in this case[1,2]. For δ-doped systems, PR spectra as well as their underlying pliysical mechanisms are still a matter of controversy a.t present[3-7].

Several attempts to interpret the PR structures observed in 6-doped samples have been based on analysis of spectral features in terms of two-dimensional (2D) electron (hole) gas for n-type (p-type) doping[3,8,9]. Although the 2D electron gas could indeed be related to the observed PR spectral features, hitherto this has not been definitively comproved from the experimental point of view. In addition, the theoretical explanation of such spectral features is still controversial.

The 6-doped structures have recently been investigated by the differential PR (DPR) technique, which allows to eliminate the surface electric field effects through the use of two laser pumps with different wavelengths[10]. However, the interpretation of the DPR spectra remains unclear, since no direct evidence of 2D electron gas contributions to the spectral line shape was exhibited.

Recently, a new tlieoretical model for optical transitions in tlie PR spectrum from δ-doped structures has been proposed by us[11]. This model is based only on tlie common 3D two-particles FK theory[12,13], and considers electric field and effective band gap variations in tlie O-region due to tlie spatially varying electron density. Such approach was applied to the single Si h-doped layer in GaAs. A good qualitative agreement between the simulated spectra[11] and experimental data[10] has been obtained.

In this paper we report on the results of application of our theoretical model[11] to two other systems, a double Si δ-doped layer structure in GaAs, and the interface between undoped and Si heavily-doped degenerated GaAs.

It is assumed that practically all electron states below the Fermi level are fully occupied, even at room

temperature, since the Fermi level is far above tlie conduction band bottom at the planar doping[7,14] or in bulk material with doping concentration of Si of order of 10^{19} cm^{-3}. Since in thcse cases the electron wave function close to tlie Fermi level is rather delocalized[7,14] and practically spread over the bulk electron coherence length[11], we can treat tlie problem of optical transitions in these structures in terms of the simplest case of two-particles FK effect.

We based our calculations on tlie well-known result derived by Aspnes and Frova[15] for the effective change of the dielectric function $< \Delta\epsilon >$ in tlie presence of nonuniform perturbations $\Delta\epsilon(\mathbf{z})$:

$$< \Delta\epsilon > = -2i\mathbf{K}\exp(2i\mathbf{K}\mathbf{z}_s) \int_{\infty}^{z_s} \Delta\epsilon(\mathbf{z})\exp(-2\mathbf{i}\mathbf{K}\mathbf{z})dz \qquad (1)$$

where $\mathbf{z}_s$ is tlie coordinate of the surface, K is tlie propagation constant and the integration interval contains the δ-region.

We have applied eq.(1) to the crise where nonuniform perturbations of the dieletric function $\Delta\epsilon(\mathbf{z})$ are due not only to an electric field ($\mathbf{F}(\mathbf{z})$) spatial inhomogenity, but also to spatial variations of tlie effective band gap energy value ($\mathbf{E}_g(\mathrm{z}) = \hbar\omega_g(\mathbf{z})$), that is

$$\Delta\epsilon(\mathbf{z}) = \Delta\epsilon(\mathbf{F}(\mathbf{z}), \omega_g(\mathbf{z})). \qquad (2)$$

This approach does not violate any assumption made in Ref.[15].

It is assumed that at any point within the δ-region or interface depletion-region the perturbation $\Delta\epsilon(\mathbf{z})$ is determined by the FK theory[12,13], using tlie electric field and effective band gap local values. We have modified the expression for At, derived by Aspnes[12] for the vicinity of tlir 3D critical point $\mathbf{M}_0$, in order to take into account the spatial variations of these parameters:

$$\Delta\epsilon(\mathbf{F}(\mathbf{z}), \omega_g(\mathbf{z})) = \mathbf{C}(\theta^{1/2}\pi/\omega^2) \{[Ai'(\eta)Bi'(\eta) - \eta Ai(\eta)Bi(\eta)] + i[Ai'^2(\eta) - \eta Ai^2(\eta)] + \eta^{1/2}\} \qquad (3)$$

where

$$\eta = (\omega_g(\mathbf{z}) - \omega + i\gamma)/\omega \qquad \theta = \mathbf{e}^2\mathbf{F}^2(\mathbf{z})/2\mu\hbar \qquad (4)$$

Here *Ai* and *Bi* are regular and irregular Airy functions, respectively, C is the normalization coefficient, w is the light photon frequency, γ is the collision broadening parameter, and μ is the reduced effective mass along the field direction.

The effective change of the dielectric function $< \Delta\epsilon >$ is directly related with tlie PR line shape as follows

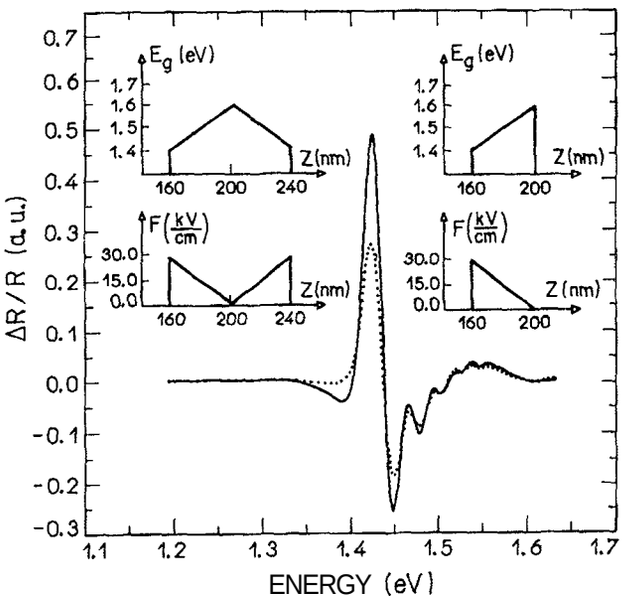
$$\Delta\mathbf{R}/\mathbf{R} = \alpha < \Delta\epsilon_1 > + \beta < \Delta\epsilon_2 >, \qquad (5)$$

where $< \Delta\epsilon_1 >$ and $< \Delta\epsilon_2 >$ are the effective changes in the real and imaginary parts of the dielectric function, respectively, and α and β are the Seraphin coefficients[15,16]. For GaAs, $\beta << \alpha$ at the vicinity of the absorption edge ($\mathbf{h}\omega_g$ = 1.42 eV for $\mathbf{T}$=300K), therefore the second term in expression ***(5)*** has been omitted[16].

The calculated DPR spectra for a single Si 6-doped layer[11] and for the interface between undoped and Si heavily-doped degenerated GaAs, at room temperature, are shown in Fig. 1. The inserts depict the effective band gap and the electric field absolute value profiles assumed, for simplicity, to he linear-type dependent on z. Only contiibutions from heavy hole-electron pairs have been consiclered. We neglect surface electric fields.

Fig. 2 shows tlie experimental DPR spectra reported by Sydor, Badakhashan and Engholm for the above systems[10]. A good qualitative agreement is observed above tlie GaAs band gap energy (1.42eV at 300K) between the theoretical curves depicted in Fig.1 and tlie experimental DPR spectra shown in Fig.2. This leads to the conclusion that the DPR line shapes of the structures under consideration could be understood in terrns of only the common two-particles FK effect, by taking into account the spatial variations of tlie electric field and effective band gap within 6- or interface region. The structure seen below the GaAs band gap in the experimental spectra of Fig. 2 does not arise from the 6- or iilterface region, since only transitions above the Fermi level are expected. We could attribute such structure to reflections from the semi-insulating/semiconductor GaAs interface[17].

The similarity between the two experimental curves, shown il1 Fig. 2, called in Ref. [10] as surprising, is quite well understood in terms of our model, once the Fermi level is far above the conduction band bottom in



Figiire 1: Calculated DPR spectra for n-type Si δ-doped GaAs (solid linc) and for the interface between undoped and Si heavily-doped GaAs (broken line). The dependences of the effective band gap value (E,) aiid of the electric field (F) on z, used in the calculations, are shown in the inserts for the δ-doped (left-hand side) and for tlie interface (right-hand side) structures. For the broadening parameter $\Gamma(\Gamma = \hbar\gamma)$ the value 0.01eV lias been used.

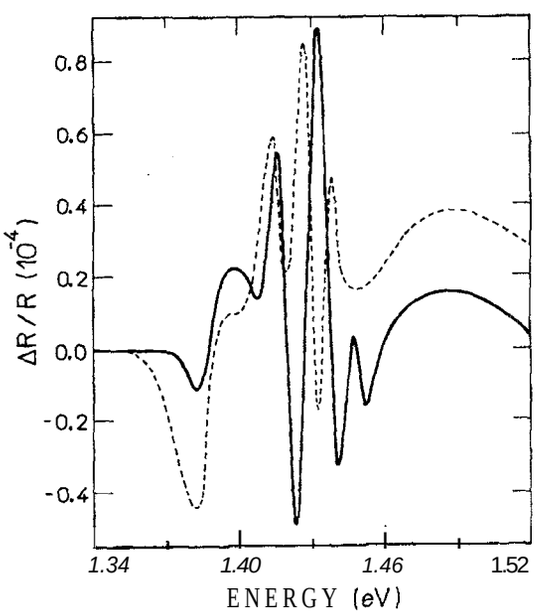


Figure 2: Observed DPK spectra from a Si δ-doped GaAs (solid line) and froni an interface between undoped and Si heavily-doped GaAs (broken line), as extracted from Ref.[10].

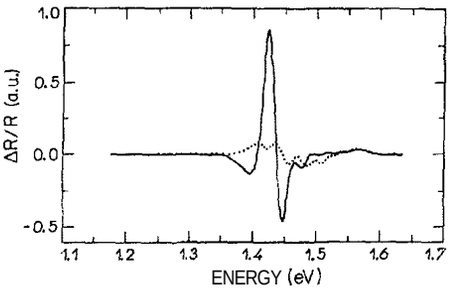


Figure 3: Calculated DPR spectra for the system containing two δ-doped layers separated hy 240nm (solid line) and 120nm (broken line). Effective band gap and electric field profiles within each 6-layer region have been introduced into tlie calculations in the same way as shown in the left-side insert of Fig.1. For tlie broadening parameter $\Gamma(\Gamma = \hbar\gamma)$ tlie value 0.01eV lias been used.

gap towards the interface takes place. This is comproved by tlie theoretical results (see Fig. I), and is also in accordance with recent PR investigations of heavily doped GaAs[18].

In Fig. **3** we show calculated DPR spectra for a δ-doped structure which contains two isolated Si 6-layers. It is worth noting that the intensity of the DPR signal is sensitive to the spatial separation between the 6-layers. Two different values for the δ-layers separation were considered in curves shown in Fig.3, which correspond to constructive and destructive interference between signals coming from tliese layers (see eq.(1)).

In conclusion, we have shown that DPR line shapes from 6-doped layers and interfaces between undoped and heavily doped materials can be calculated in terms of a.common two-particles FK effect, by taking into account the spatial variations of electric field and effective band gap in the 6- or interface region. The observed DPR spectra[10], as well as recent PR spectra. reported for a similar interface[19] as the one investigated here, may be attributed to transitions involving 3D valence- and conduction-band continuuin states above the Fermi level. In order to increase the PR signal from the discussed δ-doped structures, one can use several separated planar doped layers. However, the separation between such layers must be equal to the wavelength in the substrate (constructive interference), which corresponds to the energy of the spectral structure under examination.

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