of the spin subbands has no opportunity to become equilibrium because the spin relaxation of electrons excited high into the conduction band is being switched out at the moment of their recombination. As a result the population of the upper spin subbands occurs to be higher than expected for equilibrium conditions as it is seen from a comparison between the calculated and the experimental data in Fig. 3.

In order to estimate τ_S in the stationary case with regard to the recombination conditions in our experiment we used rate equations in the relaxation time approach assuming τ_R to be a weak function of the magnetic field:

$$\ln \{[I_\uparrow/I_\downarrow]_{exp} - [I_\uparrow/I_\downarrow]_{calc}\} = \tau_0 - (\tau_R/\tau_S), \quad (1)$$

where τ_0 is an unknown integrating constant and $[I_\uparrow/I_\downarrow]_{exp}$ and $[I_\uparrow/I_\downarrow]_{calc}$ are the experimental and calculated ratios of the PL intensities as obtained from the data in Fig. 3, respectively.

The ratio τ_R/τ_S calculated from equ. (1) is plotted in Fig. 3, too. The initial ordinate of the τ_R/τ_S curve is arbitrarily choosen to be equal τ_0. It is seen that τ_R/τ_S increases with the magnetic field and has a maximum near B = 3 T.

Thus an inverse population of the upper spin component of the lowest Landau subband connected with a nonequilibrium distribution has been observed.

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ANGLE-RESOLVED CONSTANT-INITIAL-STATE SPECTROSCOPY OF GaAs

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The conduction band energies at the Γ point of GaAs are determined experimentally in the 10 to 60 eV range by means of angle-resolved constant-initial-state measurements. The atomic orbital character and the symmetry of these states are analyzed.

1 INTRODUCTION

The experimental determination of the band structure of occupied states (valence band) of metals and semiconductors has been performed in recent years by means of angle-resolved photoemission spectroscopy (ARPES)[1)]. In most of the cases good agreement between theoretical band structure calculations and the experimental data is found. However, only a few studies have been dedicated to the unoccupied states (conduction band). Inverse photoemission [2)] and angle-resolved constant-initial-state (ARCIS) spectroscopy [3)] have delivered experimental points for GaAs up to approximately 15 eV above the valence-band-maximum (VBM). In the present work we show ARCIS experiments on GaAs at the Γ point up to 60 eV above the VBM and compare the data with empirical-pseudopotential-method (EPM) calculations. The atomic orbital character and the symmetry of the states are also considered.

ARCIS measurements were performed at room temperature with a Toroidal Energy Analyzer [4)] at normal emission. The angular resolution was ±1° and the combined analyzer-monochromator resolution better than 0.25 eV. The base pressure in the measurement chamber was 1×10^{-10} mbar. Monochromatized light was delivered by a Toroidal Grating Monochromator (TGM4) at the Synchrotron Radiation facility BESSY (Berlin).

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2 RESULTS

In Fig.1 we show ARCIS spectra for transitions arising from the VBM (Γ_{15}^v) (Fig.1a) and from the valence-band-minimum (Γ_1^v) (Fig.1b). All energies are referred to the VBM. Features associated with direct transitions at Γ are represented by E_0, less prominent features (shoulders) by S, and R accounts for resonances associated with core lines. We concentrate our analysis here mostly on the E_0 features. A more detailed analysis can be found in Ref.(5). In the present work we compare the measured data with EPM calculations [6] and with our own calculations using the Cohen-Bergstresser method with the pseudopotential form factors of Ref.(7) and a basis set of 89 plane waves. Next, we compare both calculations with the experimental points, which are listed in Table I.

In the energy range up to 15 eV above the VBM, we observe resonable agreement between the theoretical calculations and the experimental data, the maximum difference being about 2 eV. Features $E_0(av.)$, $E_0'(av.)$ and $E_0'''(av.)$ are taken from electroreflectance measurements [8] and E_0^{IV} and E_0^V from Ref's.(3,5). The first significant difference between the calculations is found at about 22.60 eV. In this case only Ref.(6) predicts E_0^{VI} correctly. At higher energies severe discrepancies between our calculations and the experimental data are observed. No bands in this range are given in Ref.(6). However, the discrepancy can be reduced if the theoretical bands are shifted towards higher energy by about 6-8 eV.

A more rigorous assignment of individual final states to a particular transition can be made if one considers the symmetry of the final states. The initial states Γ_{15}^v and Γ_1^v have $4p$ and $4s$ character, respectively. According to the transition selection rules [9], transitions from Γ_{15}^v to Γ_1^c ($s-$ or $f-$like), Γ_{12}^c ($d-$like), Γ_{15}^c ($p-$, $d-$ or $f-$like) and Γ_{25}^c ($f-$like) are possible. From Γ_1^v only transitions to Γ_{15}^c are allowed. With the atomic orbital sequence and the corresponding symmetries we identify the measured features. E_0^{VI}, which is reached from Γ_1^v (Fig.1b) as well as from Γ_{15}^v [5], has $5p$ character and Γ_{15} symmetry. After the shift of the theoretical bands by about 6 eV we identify E_0^{VII} as a $4d^*$ state with Γ_{12} symmetry, E_0^{VIII} with $4d^*$ and Γ_{15}, and E_0^{IX} with $5p^*$ and Γ_{15}. The star represents an anti-bonding atomic orbital. Note that E_0^{VII} is not observed in Fig.1b because it has Γ_{12} symmetry. However, E_0^{VIII} is not identified in Fig.1a, a fact that is not yet understood. Feature S_3, which was identified as a possible plasmon loss peak [5], corresponds to a $6s$ state

(Γ_1). E_0^X and E_0^{XI} are further identified as $6p$ and $6p^*$ states, respectively, both with Γ_{15} symmetry. Both features are clearly seen in Fig.1b because from Γ_1^v the p-like final states have the strongest probability, but they appear only as shoulders in Fig.1a because from Γ_{15}^v the p-like final states posess the lowest probability. The same argument accounts for the opposite behaviour of S_6 (d-like). We thus conclude that the identification of the symmetries of the final states is compatible with the transition selection rules.

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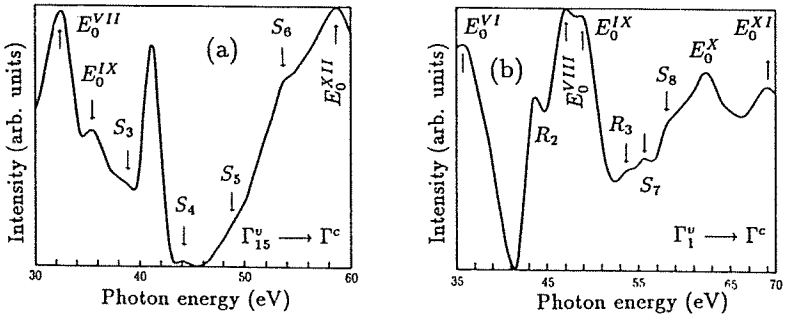

Fig.1. Normal emission ARCIS spectra of GaAs(110) surfaces for initial states at: (a) Γ_{15}^v and (b) Γ_1^v.

atomic orbital character	symmetry	energies (eV) experiment	EPM Ref. (6)	EPM This work	transitions observed from Γ_{15}^v	from Γ_1^v
4s	Γ_1	−13.25	−12.40	−12.10	–	–
4p	Γ_{15}	0.00	0.00	0.00	–	–
4s*	Γ_1	1.63[8]	1.65	1.48	E_0 (av.)	–
4p*	Γ_{15}	4.72[8]	4.81	4.43	E_0' (av.)	–
5s	Γ_1	8.33[8]	6.88	8.36	E_0''' (av.)	–
4d	Γ_{12}	10.53[8]	9.99	8.90	E_0'' (av.)	–
		10.60[3]				
		10.72				
4d	Γ_{15}	12.80[3]	12.09	13.30	E_0^{IV}	–
		12.60				
5s*	Γ_1	14.90[3]	12.86	14.50	E_0^V	–
		15.20				
5p	Γ_{15}	22.62	22.60	27.00	E_0^{VI}	E_0^{VI}
4d*	Γ_{15}	34.13	–	27.70	–	E_0^{VIII}
4d*	Γ_{12}	32.38	–	27.90	E_0^{VII}	–
5p*	Γ_{15}	35.61	–	28.50	E_0^{IX}	E_0^{IX}
6s	Γ_1	39.50	–	28.70	S_3	–
6s*	Γ_1	43.86	–	39.6	S_4	–
6p	Γ_{15}	49.43	–	41.30	S_5	E_0^X
5d	Γ_{12}, Γ_{15}	52.00	–	42.70	S_6	–
5d*	Γ_{12}, Γ_{15}	58.61	–	44.90	E_0^{XII}	–
6p*	Γ_{15}	55.67	–	51.4	–	E_0^{XI}

TABLE I: Comparison of the measured values of E_0 features from this work and Refs. (3,8) with EPM calculations from Ref. (6) and this work. The atomic orbital character and the corresponding symmetry is also shown.

THE TEMPERATURE DEPENDENCE OF THE INDIRECT BAND GAP OF SILICON: THEORY AND FIRST-PRINCIPLES CALCULATION

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It is widely believed that the major part of the temperature dependence of the band gap of semiconductors normally arises from electron-phonon interactions. In this paper we present results from a first-principles calculation of the electron-phonon contribution to temperature dependence of the minimum indirect band gap of silicon, and comment on some of the qualitative features of the theory.

INTRODUCTION

The theory of the electron-phonon (el-ph) contribution to the temperature dependence of the band gap, $\Delta E_g(T)$, has a long history dating back to the work of Fan,[1] Brooks[2] and Antoncik.[3] The effects of the el-ph interaction can be interpreted as causing the phonon frequencies of the solid to be a function of the electron occupation. As a consequence excitation of an electron from the valence to the conduction band of a semiconductor is accompanied by a change in the phonon spectrum of the solid and a change in the energy stored in the phonon degrees of freedom. This energy is seen experimentally as a temperature dependent shift in the band gap. In the case of an optical excitation which takes an electron from Bloch state |kn> to |k'n'> we have[1,4,5]

$$\Delta E_g(T) = \sum_{qj} \hbar \left(\delta\omega_{qj,kn} - \delta\omega_{qj,k'n'} \right) n\left(\omega_{qj}, T \right) \qquad [1],$$

where ω_{qj} is the frequency of the phonon with wavevector $\mathbf{q}$ in branch j, $\delta\omega_{qj,kn}$ is the change in the phonon frequencies of mode $\mathbf{q}$j caused by adding an electron to state |kn>, $n(\omega_{qj},T)$ is the Bose occupation factor, and where the sum over $\mathbf{q}$,j runs over all the phonon modes of the system. Equation [1] plays a central role in our first-principles determination of the temperature dependence of the gap which proceeds by direct evaluation of the terms on the right hand side of [1]. Note that for a system with extended electron and phonon modes each phonon frequency change, $\delta\omega_{qj,kn}$, will be of order $(1/N_{at})$ where N_{at} is the number of atoms in the solid. It is therefore convenient to introduce a phonon hardening parameter, α_{qj}, defined by[4,5]

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CONTENTS

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