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Electronic structure and photoemission spectra of thin $(GaAs)_n(AlAs)_n$ superlattices

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Abstract

Increased translational period of crystalline superlattices gives rise to qualitative modifications of the electron band structure $E(k)$: minigaps appear at new Brillouin zone boundaries and band dispersions are reduced into narrower allowed energy bands. Modifications of the wave functions, consisting in electron confinement into one of the two components of a superlattice can affect the intensities of photoemitted electrons. The layer-resolved contributions from a few topmost layers to the photoelectron intensity are evaluated in the one-step model and the importance of the related optical matrix elements is shown. Large number of surface states and resonances connected with superlattice can be expected. This expectation is confirmed by evaluation of the local densities of electron states for the unreconstructed (1 0 0) surface of the 2×2 superlattice. The space distribution of localized states is presented. Energy distribution curves for normally photoemitted electrons are analyzed from the above viewpoints.

Keywords: Electron density, excitation spectra calculations; Green's function methods; Angle resolved photoemission; Photoelectron emission; Gallium arsenide; Low index single crystal surfaces; Superlattices

1. Introduction

In contrast to usual crystals with their well-known translational periodocity crystal superlattices have additional translational periodicity in one direction. This longer period is introduced artificially by the alternate deposition of individual components (e.g. in the molecular beam epitaxy). For a binary superlattice this new periodicity is given by the layer thicknesses of the two components. In a simple case when the lattice constants of the two components can be considered the same, the new translational period is given by the numbers of atomic layers in these components. This situation is encountered in systems composed of GaAs and AlAs: $(GaAs)_n(AlAs)_n$ denotes a superlattice with repeatedly alternating n layers of GaAs with n layers of AlAs in the [1 0 0] growth direction.

The reduced translational symmetry of a superlattice implies corresponding decrease of the dimension of the Brillouin zone in this direction and the new zone boundaries lead to opening of the gaps in the electron dispersion relation $E(k)$: superlattice minigaps [1].

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Electron confinement effects in semiconductor superlattices have been first reported in long-period superlattices. The spatial confinement at energies close to the maingap [2] is a direct consequence of the confinement at a single interface between two crystals where the valence band offset at the GaAs/AlAs interface ensures that the states from the top of the valence band are localized in the GaAs region. The long-period superlattices can be adequately described by means of the envelope function where each layer is considered as a macroscopic crystal modified at most by a slowly varying potential. These confinement effects have been found in model studies and the preferential confinement to interfaces has been related to electron localization to isolated interfaces (interface states [1]). They have been observed in medium-period superlattices [3] and even in short-period superlattices [4].

The case with a crystal potential superimposed by a longer period additional potential has been studied in detail by Slater [5] on a one-dimensional model with sinusoidal potentials. Apart from qualitative modifications of the electron energy spectrum spatial distribution of electrons has been analyzed: confinement effects consisting in predominant localization in different regions within the long period have been reported. These effects have been shown to take place in the whole bands or only at energies close to the newly created minigaps depending on the magnitude of the imposed longer period potential (as reflected in the ratio of the width of the minigap to the width of the original band).

Here, we will study confinement effects around minigaps created in very-short-period superlattices $(GaAs)_n(AlAs)_n$. Apart from the bulk effects, the role of the surface will be considered: for an ideally terminated (1 0 0) surface confinement effects in the valence band and their role in determining the intensities of electrons photoemitted from these superlattices will be investigated.

2. Theory

Because substantial part of the photoemission comes from superlattice surface layers the photocurrent is calculated within the one-step model. The initial states are represented by a half-space Green's function. The basis set consists of the 4s and 4p atomic orbitals of gallium and arsenic and the 3s and 3p atomic orbitals of aluminum. The associated Hamilton matrix is calculated according to the Extended-Hückel-Theory. The parameters for GaAs and AlAs are adjusted to give correct value of the valence band offset 0.45 eV between GaAs and AlAs. The final state of photoemission is a time reversed LEED state determined by matching the solution of the complex band structure to the vacuum solution, representing the surface by a step potential. For more details the recent paper [6] and references there are to be used.

3. Results and discussion

In this section results for the ideal $(GaAs)_2(AlAs)_2$(0 0 1)-(1×1)Ga surface, i.e. Ga-terminated superlattice are presented. We will concentrate our investigation to the centre of the surface Brillouin zone $\overline{\Gamma}$. We have a quasi-one-dimensional problem related to the one-dimensional model studied by Slater [5]. The superlattice period is two times longer than that for its components (period a) and the corresponding Brillouin zone dimension becomes four times shorter: $\Gamma Z = 1/4\Gamma X$.

Numerous gaps within the valence band are responsible for splitting of original bulk dispersive branches into smaller segments with dispersions limited to the narrower minibands of a superlattice. Dispersive peaks characteristic for bulk transitions become thus less pronounced in angular resolved photoemission and it is more difficult to distinguish bulk states from surface states (with no dipersion).

The energy band structure of the superlattice is simpler in the lower half of the valence band (derived from the light-hole band of GaAs) because of the absence of intervening heavy-hole derived bands here. Rather large minigap, situated from -6 to -5 eV has been found [6,7] and Fig. 1 shows electron confinements in the bands just below and above this minigap.

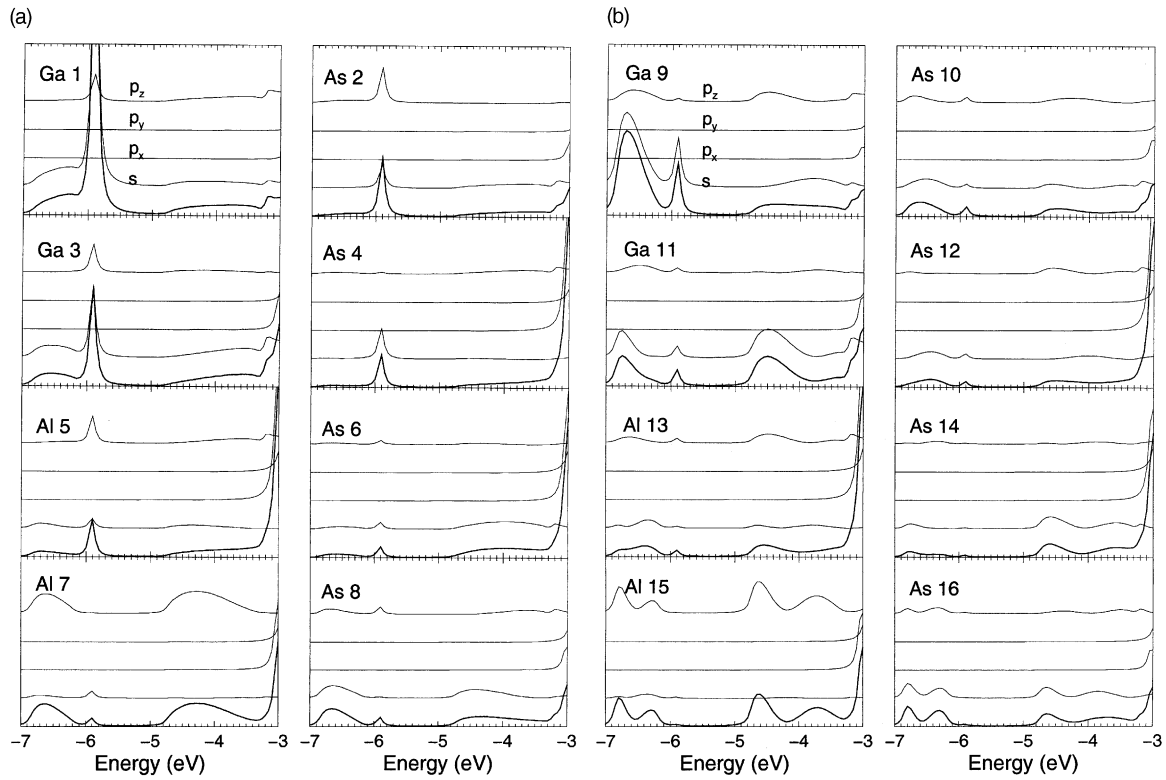

Fig. 1. Layer- and orbital-resolved density of states for $(GaAs)_2(AlAs)_2$-(1×1)Ga superlattice at the $\overline{\Gamma}$ point for the topmost eight atomic planes (a), for the next eight atomic planes (b) and for the eight atomic planes in the bulk (c). Energy is referred to the top of the valence band.

At the lower edge of the minigap a surface state is observed with a typically slow decay into the bulk. Generally, the number of surface states in superlattices gets increased in comparison with crystal component surfaces [6]. Their slow attenuation into the bulk makes their difference from bulk states to be diminished, however.

Fig. 1c shows local densities of electron states within one superlattice period for the bulk. As there is only very small contribution from As atomic layers we can concentrate on cation layers (left). The electron confinement expected from Slater's model is partially confirmed here. Major concentration of the states from below the gap is seen to occur on one of the two interfaces between GaAs and AlAs, the region above the gap is mostly void. On the other hand, the other interface displays a weak enhancement of the local density of states above the minigap. Much stronger asymmetry of the above type is seen in the surface region, Fig. 1a (surface state contribution dominates around −6 eV). The subsurface region, Fig. 1b, shows a gradual transition to the bulk behaviour.

Electron confinement (wave function localization in the direct space) in the vicinity of minigaps can be understood as a formation of a standing wave in analogy to the well-known formation of sine and cosine waves next to the gap in the nearly free electron approximation. It is taken into account in photoemission by means of optical matrix elements between the initial and final states. These matrix elements govern the intensity of photoemitted electrons similarly as e.g. the symmetries of initial and final states. Because of the short electron mean free path (of the order of superlattice periods) we can expect that the contribution to the emitted intensity will be substantially decreased

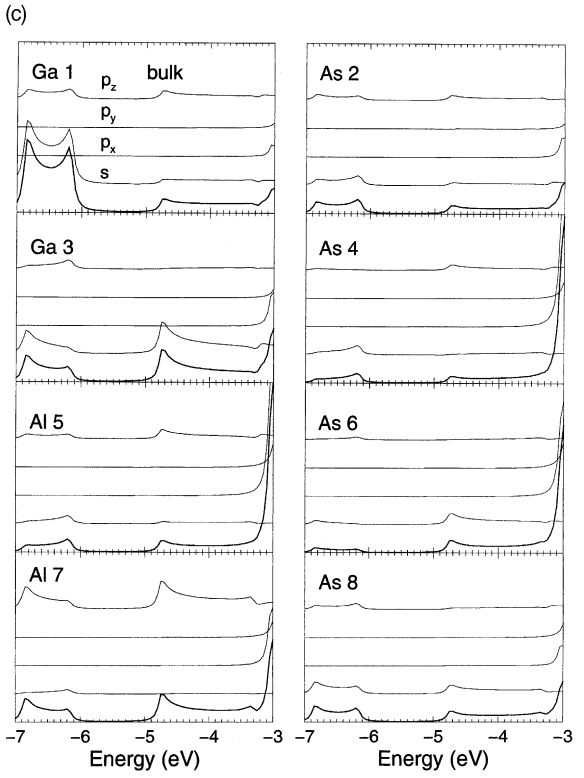

Fig. 1 (*continued*)

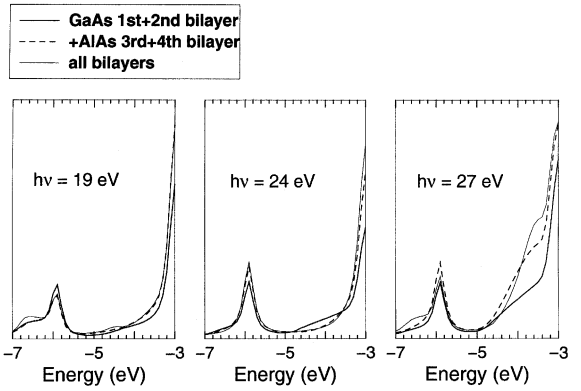

Fig. 2. Layer-resolved and layer-integrated photocurrent (normal emission) for $(AlAs)_2(GaAs)_2(0\,0\,1)$-$(1 \times 1)$Ga, calculated for three different photon energies. The spectra are not broadened with an experimental resolution and were not multiplied by a Fermi distribution. Thick solid lines represent the photocurrent from the first two GaAs bilayers, while the thick dashed lines show the photocurrent integrated from the first two GaAs and AlAs bilayers. The thin lines illustrate the contribution of all 36 bilayers, taken into account in the calculation.

if the occupied electron states are confined to deeper lying layers of a superlattice and enhanced if the contributing states are confined to regions close to the surface.

In Fig. 2, the normally photoemitted electron current is shown decomposed according to the origin of the excited electrons. The energy range corresponds to the vicinity of the minigap discussed above. Apart from a decreased intensity within the minigap, (except just above the lower gap edge where surface state dominates) very small intensity at energies above the minigap is clearly seen which is in agreement with the electron confinement there (Fig. 1). For energies below the minigap the topmost period contribution clearly dominates for all three excitation energies. This behaviour contrasts with that illustrated for a peak at −2.2 eV (no confinement) in our previous study [6] where rather different composition for three excitation energies is observed. Thus, the electron confinement has a dominant role in determining the photoemission intensity at energies close to the minigap.

4. Conclusion

Electron confinement has an important role in determining the electron band structure of crystalline superlattices. Apart from confinement effects due to the valence band offsets in semiconductor superlattices confinement effects in the vicinity of the minigaps have been found and interpreted. These effects may serve as a qualitative tool in predicting intensity changes in the energy distribution curves of electrons photoemitted from superlattice surfaces. The surface sensitivity of the photoelectron spectroscopy makes it suitable for the investigation of electron confinement effects. Interpretations of the intensities requires theoretical calculations based on the one-step model of photoemission.

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