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ELECTRONIC STRUCTURE OF SEGREGATED Ge-(110) GaAs OVERLAYER SYSTEMS

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In this paper we report the first electronic structure calculation for a Ge-(110) GaAs overlayer system (OS) in which the recently reported segregation of As to the surface of the OS was taken into account. The calculations were carried out using the tight binding scattering theoretical method. The OS band structure as well as angular resolved layer densities of states are discussed and compared with our previous results for ideal (110) overlayer systems. We find that Ge-(110)GaAs overlayer systems show a number of distinct interface-induced electronic features, which should be directly accessible to ARUPS experiments.

Interfaces in semiconductor heterostructures have been the subject of intensive theoretical investigations during the past several years [1]. On the contrary, much less experimental information on the *microscopic* electronic properties of semiconductor interfaces was reported up to date. One of the reasons for the lack of more experimental data certainly lies in the fact, that the most appropriate tool for such studies, namely angular resolved ultraviolett photoelectron spectroscopy (ARUPS), can not directly be applied to heterojunctions (two very thick, i.e. semiinfinite, solids in contact) because of the very small escape depth of the photoexited electrons. The interface between two semiconductors is only accessible to ARUPS measurements if at least one of the two materials is in the form of a thin overlayer, a few Å thick. Using such systems as samples poses the question wether they can yield information about true heterojunction interface properties. This question has been investigated for *ideal* Ge-(100)GaAs and Ge-(110)GaAs overlayer systems by Pollmann and Pantelides [2] and by the present authors [3], respectively. Both studies showed, that three Ge overlayers on semiinfinite GaAs are sufficient in order to reproduce all characteristic *heterojunction* interface electronic features in the *overlayer system*. ARUPS experiments, which could verify these predictions, are still lacking. Denley et al. [4] carried out photoemission measurements on overlayer systems but they used (110) GaAs with submonolayer coverage of Ge as samples so that their data can not directly be compared with our results. Recently, Mönch and Gant [5] reported AES, LEED and CPD investigations of a variety of Ge-(110) GaAs overlayer systems ranging from submonolayer Ge coverage up to a hundred monolayers of Ge. These authors observed *segregation* of As from the interface to the surface of the overlayer system. In consequence, the GaAs layer next to the interface becomes depleted from As with Ge atoms substituting for the As atoms at the interface layer. In this paper we report electronic structure calculations in which the experimentally observed As segregation was taken into account to a certain extent. The model, which we have investigated, is shown in Fig.(1). We have retained the ideal lattice geometry up to the surface [6]. The system depicted in Fig.(1) differs from an ideal 3Ge - (110) GaAs overlayer system only in that all As atoms at the GaAs interface layer have been interchanged

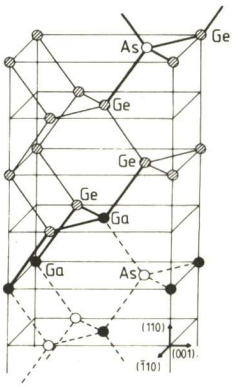

Fig. 1

with Ge atoms from the surface layer. This is certainly an idealized model in the sense that such discontinuous stoichiometry changes are unlikely to occur in a real sample. A system with, e.g., a continuously varying As distribution on the outermost layers can not be treated by the presently available theoretical techniques. We believe, however, that a more continuous change in the As distribution near the surface and in the Ge distribution near the interface would not yield very drastic changes in the resulting spectra since no entirely new types of bonds would be created.

The calculations have been carried out using the scattering theoretical method for interfaces [7]. We have used the same tight binding bulk Hamiltonians and interface interaction matrices as employed in our studies of the heterojunction interface [8] and the ideal overlayer sytems [3]. Our heterojunction interface results were discussed in [8], and were found to be in very good overall agreement with the selfconsistent calculations of Pickett, Louie and Cohen [9].

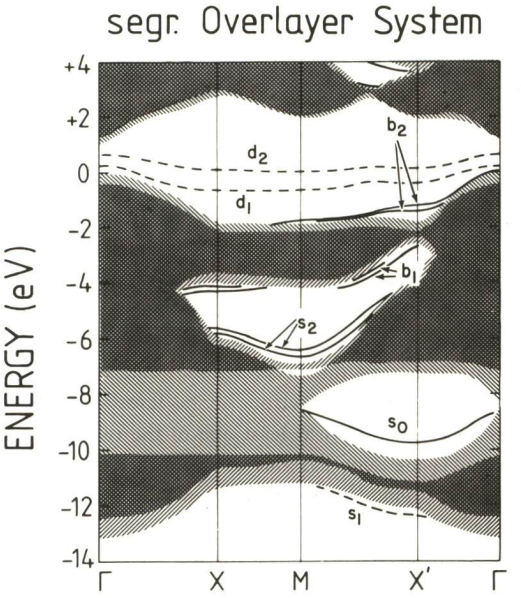

Fig. 2 Joint projected band structure and bound states for the segregated 3Ge - (110) GaAs overlayer system

In Fig.(2), we show the electronic band structure for the segregated overlayer system. The shaded areas show the joint projected band structure for Ge(\\\) and GaAs(///), respectively. Bound states of the OS are shown by dashed or full lines. The surface and interface bands shown in the figure can be interpreted very intuitively by referring to the changes in the binding environment at the surface and at the interface, respectively, as compared to the corresponding bulk situation. In general, Ge-As bonds are stronger and Ge-Ga bonds are weaker than either Ge-Ge or Ga-As bulk bonds. In consequence the Ge-As and Ge-Ga bonds depicted in Fig.(1) give rise to bound states which occur below (s_1, b_1) or above (s_0, s_2, b_2) the respective bulk bands from which they are derived. We have used lower case letters for labelling the various states in order to avoid confusion with our results for the ideal overlayer system [3]. While we found only one S_2, B_1 and B_2 band for the latter, we find a group of two slightly split bands in each case, now. The two split bands result from the two different kinds of Ge-Ga or Ge-As bonds, respectively, found in the segregated OS. In the *ideal* OS, there exist only Ge-Ga and Ge-As bonds that *connect neighbouring* (110) layers. In the *segregated* OS, we have in addition Ge-Ga and Ge-As bonds which *lie in* the surface or *in* the interface layer, respectively (see Fig.(1)). The latter give rise to states that are slightly split from the former. All dashed lines show bound states which are localized at or near the surface. The bands d_1

and d_2 result from As and Ge surface dangling bond states, respectively, and the band labelled s_1 results from the Ge-As bonds at the surface. It is a surface back bond state in nature. A more detailed analysis of the wavefunctions will be given elsewhere [10].

In addition to the bound states, the new bonds at the interface and surface give rise to more or less pronounced resonances. We have calculated wavevector-resolved layer densities of states at the Brillouin zone center for the segregated overlayer system and have summed up these LDOS's layer by layer, weighted by an exponential decay factor using 7 Å as decay length. The resulting angular resolved weighted LDOS is given in Fig.(3). It corresponds to normal emission ARUPS spectra in the simplest approximation. The corresponding result for the *relaxed* (110) GaAs surface (which would be the reference sample for an experimental investigation of a variety of overlayer systems) is shown as well in Fig.(3). For comparison we give in Fig.(4) the ARWLDOS at the zone center for the ideal 3 Ge - (110) GaAs overlayer system, which was discussed in Ref. [3]. First we note, that the introduction of new bonds at the interface gives rise to a number of very pronounced features in the ARWLDOS. Since both the segregated as well as the ideal OS's have the same kinds of new bonds (Ge-Ga and Ge-As) in addition to the Ge-Ge and Ga-As bulk bonds, the new spectral features are grossly similar in both cases. However, the number of changed bonds near the surface and near the interface is different in the segregated system as compared to the ideal system. Therefore, the relative intensity of the various spectral peaks in Fig.(3) is very different from that in Fig.(4). The peaks 1 through 7 in both Figs.(3) and (4) have essentially the same origins. Peaks 1, 3 and 7 are predominantly due to GaAs bulk states. Peaks 2 and 5 are Ge derived and result from states that are mainly localized in the overlayers. The peaks 4 and 6 originate from Ge-As and Ge-Ga bonds, respectively. It should be noted that the spatial distribution of these states is different in the segregated OS as compared to the ideal OS, since the Ge-As bonds do no longer occur at the interface (see Fig. 1). Only the peak 1' in Fig.(3) is completely new and thus characteristic for the *segregated* OS. It results from the Ge-As surface back bond states which are absent at the ideal OS. A more detailed discussion will be given in [10].

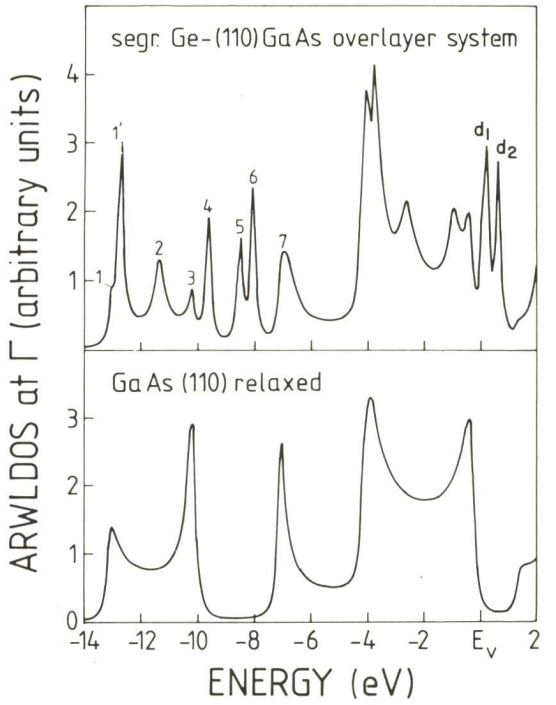

Fig. 3 Angular resolved weighted LDOS at the Brillouin zone center for the segregated overlayer system (broadened by 0.1 eV)

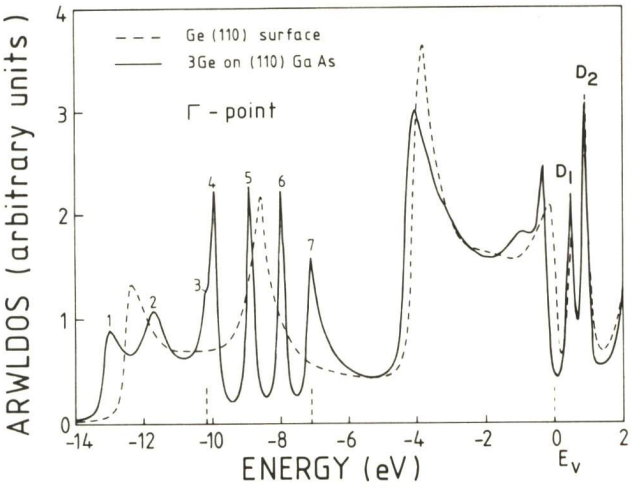

Fig. 4 Angular resolved weighted LDOS at the Brillouin zone center for the ideal 3 Ge-(110) GaAs overlayer system (broadened by 0.1 eV)

Our results for the segregated overlayer system confirm the general notion, that the electronic structure of interfaces in heterojunctions or overlayer systems can be interpreted in a straigtforward way in terms of changes in bonds as compared to the bulk binding environment. In conclusion, the new bonds at the interface of overlayer systems give rise to very pronounced, fingerprint-like spectral features, which should make these systems useful as samples for experimental investigations of semiconductor interface properties.

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