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Electronic structure of buried Si layers in GaAs(001) as studied by soft-x-ray emission

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It is demonstrated that it is possible to investigate details of the electronic structure of an internal atomic monolayer using soft-x-ray-emission spectroscopy. The local and partial density of states of one monolayer and three monolayers of Si, embedded deep below a GaAs(001) surface, was extracted. Clear differences to the density of states for bulk Si were observed.

INTRODUCTION

Knowledge of the electronic structure of internal layers and their interfaces is a key concept for understanding the properties of semiconductor devices. Yet very little has been published in this area due to lack of suitable experimental techniques. The electronic structures of clean surfaces and thin overlayers have been investigated extensively using mainly photoelectron spectroscopy. As the probing depth of this and related techniques is limited to a few atomic layers, they are not useful for the examination of buried layers. Methods which probe the volume of materials have also not been applied, because it has generally been thought that the signal from a small volume, such as a buried monolayer, would be below the noise level.

Soft-x-ray-emission spectroscopy (SXES) offers both elemental and chemical information due to the involvement of both core and valence states. Moreover, it has the ability to probe appreciable depths of the sample. The use of high brightness synchrotron radiation sources has opened research areas previously not accessible for SXES. This allows one to study, for instance, adsorbates of monolayer thicknesses, taking advantage of the ability of SXES to separate the adsorbate contribution to the valence band from that of the substrate.[1] Likewise, it is possible to detect a buried layer due to the appreciable penetration of soft x rays.[2] In the present work we have applied synchrotron-radiation-excited SXES to study the electronic structure of buried monolayers.

EXPERIMENT

It has been shown that coherently strained ultrathin Si films can be embedded in GaAs(100).[3] The heterostructures were grown by solid source molecular-beam epitaxy on GaAs(100) substrates. After standard growth of a buffer layer, exhibiting a (2×4) surface reconstruction, the substrate temperature was set to 500 °C and Si was deposited at a rate of 1 ML/1000 s. At this growth temperature only a limited diffusion of Si into GaAs is expected. The Si layer was finally capped by a 100-Å-thick GaAs layer, grown at the same temperature.

The SXE experiments were carried out at beam line 7.0 of the Advanced Light Source at Lawrence Berkeley Laboratory. This beam line comprises a 99-pole 5-cm undulator and a spherical grating monochromator.[4] Refocusing is done with Kirkpatrick-Baez-type grazing incidence optics yielding a small beam spot (<50 μm), which is of great importance for the present type of experiment. The resolution is that of the undulator peak at 140 eV, about 3 eV. The soft-x-ray emission was measured by a grazing incidence spectrometer.[5] The main features of the instrument are an arrangement of fixed gratings and a large position-sensitive array detector. The entire instrument is flange mounted on an analysis chamber (which can be rotated 90° around the incoming beam under UHV conditions, making angle-resolved SXES feasible). The system includes provisions for load-lock sample introduction and transfer.[6] The ultimate resolving capability of the instrument (about 2000 depending on energy) is determined by the spatial resolution of the 40-mm-diameter detector, which is 100 μm. In the present experiments the resolution of the spectrometer was set to 0.4 eV.

RESULTS AND DISCUSSION

Figure 1 displays soft-x-ray-emission spectra from bulk Si and bulk GaAs samples and from buried Si structures, 1 ML Si/GaAs and 3 ML Si/GaAs, respectively. The Si $L_{2,3}$ spectrum has been extensively studied and can be found in literature.[7] It can be interpreted simply in terms of partial valence-band density of states (DOS) weighted by transition probabilities. Peaks A and B are associated with s partial DOS and can be interpreted within the commonly used sp^3 model. Peak A can be viewed mainly as a tight-binding formation of the $3s$ atomic states, while peak B also involves strong hybridization effects with the Si $3p$ states. The broad feature C goes beyond the sp^3 model and arises from rather weak s and d partial DOS.[8] Although this partial DOS is quite low, it is observed with significant intensity due to a large d to p transition probability.

The GaAs spectrum has to our knowledge not been published before and has a different interpretation. The peaks D and E originate from the Ga quasicore $d_{3/2}$ and $d_{5/2}$ states appearing just below the bottom of the GaAs valence band. From the band structure of GaAs,[9] we expect in principle a Ga s valence-band contribution around 6 eV below the top of the valence band at F. There is possibly some faint structure

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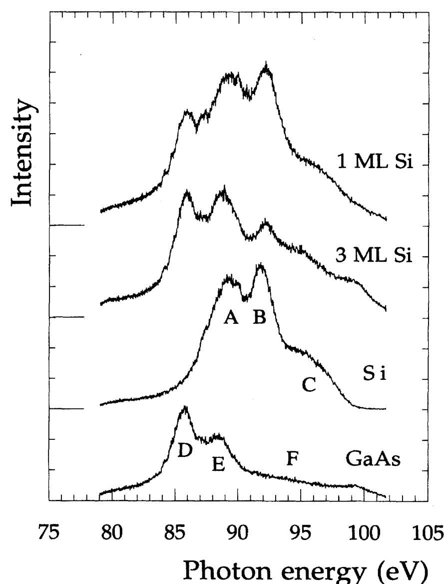

FIG. 1. Soft-x-ray-emission valence-band spectra from $L_{2,3}$ Si in bulk Si, Ga, $M_{4,5}$ in bulk GaAs, and from heterostructures with 1- and 3-ML-thick Si layers 100 Å below the GaAs(100) surface. Photons of 120 eV were used for excitation.

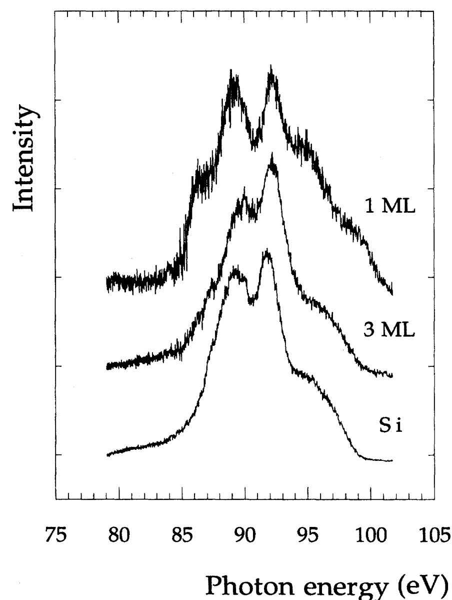

FIG. 2. The SXE $L_{2,3}$ spectrum of Si compared with difference spectra obtained by subtracting the Ga $M_{2,3}$ spectrum of bulk GaAs from the 1- and 3-ML Si/GaAs heterostructure spectra (see text for details).

there, but much weaker than the dominating *d* contributions.

Unfortunately, the Si $L_{2,3}$ and Ga $M_{4,5}$ levels have almost the same binding energy and thus the two valence-band emission spectra overlap strongly. In the heterostructure spectra all the main features of the bulk Si and bulk GaAs spectra are found. Note that the Si layer contribution is of the same order of magnitude as the GaAs contribution. To extract the Si layer contribution we applied a simple subtraction method. In this procedure the GaAs spectrum was scaled so that the two strong Ga peaks *D* and *E* were completely removed in the difference spectrum. The results are shown in Fig. 2. For the 3-ML spectrum a 0.26-eV shift of the high-energy edge, as compared to the bulk Si spectrum, is found. This effect is probably not a change in the valence-band width because the change in the threshold energy is the same. More likely it arises from a Si chemical core-level shift due to the neighboring As atoms. Correction for this effect does not, however, remove the observed depletion in the DOS at the bottom of the difference spectrum. For the 1-ML spectrum the two Ga *d* peaks could also be completely removed by the subtraction procedure. Here, however, a new peak appears around 86 eV. We interpret this as a hybridizing effect between the Si *s* states with the As *s* states. The latter appear about 12 eV below the valence-band top in GaAs.[9] It is reasonable that the DOS of the 1-ML Si layer deviates more from bulk Si DOS than the 3-ML Si DOS does.

Further studies are in progress which include near-threshold measurements, detailed analyses of the geometrical structure of the internal layers, and electronic structure calculations.

CONCLUSIONS

This investigation demonstrates that it is feasible to study details of the electronic structure of internal ultrathin layers using SXES. Si local, *s-d* partial DOS were extracted in the case of 1- and 3-ML Si layers deep inside a GaAs sample. Clearly detectable differences as compared to the bulk Si DOS are observed. For the 1-ML case the GaAs states are found to mix strongly into the Si states while for the 3-ML Si layer this effect is small.

ACKNOWLEDGMENT

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