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Insight into the local density of states at Si sites at the submonolayer Si/Ge(001)-2 × 1 interface from Si KLV Auger spectroscopy

P Unsworth and P Weightman

Surface Science Research Centre and Department of Physics, University of Liverpool, Liverpool L69 3BX, UK

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Abstract

An analysis of the differences observed between the Si KLV Auger spectra of the Si/Ge(001)-2 × 1 interface and pure Si indicates that the electronic structure of the interface is characterized by a reduction in the local p DOS at the Si sites and a transfer of p valence charge from Si to Ge. As a result, the screening of core-ionized Si sites at the interface is significantly shifted towards s screening compared with the situation for pure Si. It is possible that there is an increase in the on-site electron correlation energy, U_P, for Si sites at the interface as compared with pure Si.

1. Introduction

Semiconductor devices based on Si/SiGe heterostructures have become a small but significant percentage of manufactured semiconductor devices and this percentage is expected to increase as SiGe is used in complementary metal oxide technology [1, 2]. These developments draw attention to the need to understand the local electronic structure of Si/Ge interfaces. As discussed by Jenkins and Srivastava [3] the submonolayer growth of Si on the Ge(001)-2 × 1 reconstructed surface [4, 5] has received less attention than its counterpart the growth of Ge on the Si(001)-2 × 1 interface [6, 7]. Studies by Jesson *et al* [4] found that the growth of Si on a Ge(001)-2 × 1 surface held at 623 K produced a sharp 2 × 1 Si dimer overlayer structure. Scanning tunneling microscopy (STM) studies by Wulfhekel *et al* [5] have shown that submonolayer overlayer growth of Si at 623 K on the Ge(001)-2 × 1 surface produces four different arrangements of Si dimers but does not produce isolated Si surface atoms. The thermodynamics of these systems has been studied recently by Leite *et al* [8].

Insights into the electronic structure of such overlayer structures would complement the information that has been obtained on their physical structure and provide useful information for the understanding of heterojunction Ge/Si semiconductor devices. Electron spectroscopy techniques have the potential to reveal information on the local electronic structure of an interface provided the interface is sufficiently shallow for the electrons to escape the material. Unfortunately the direct probe of the electronic structure of an interface by photoelectron spectroscopy of the valence bands is often unsatisfactory since the valence band spectra are often dominated by the contribution from the valence bands of the bulk materials and the changes induced in the local electronic structure at the interface usually make only a weak contribution to the spectrum. We have shown that Auger spectroscopy can reveal details of the local electronic structure of the As/Si(100) and As/Si(111) interfaces that are important in attempts to integrate GaAs and Si technologies [9, 10]. In this work we apply Auger spectroscopy to a submonolayer coverage of Si on Ge(001)-2 × 1. We show that an analysis of the Si KLV Auger spectra reveals a significant reduction, compared to pure Si, in the screening of core-ionized Si sites by the local valence p density of states (DOS) compared to the local valence s DOS. This indicates a substantial corresponding change in the local DOS on Si sites in the ground state at the interface.

2. Experimental details

The experiments were carried out in an ultra-high vacuum (UHV) chamber with a base pressure of 4×10^{-11} mbar attached to a high performance Auger and x-ray photoelectron spectrometer equipped with a monochromated Al Kα and a Ti x-ray source [11]. The Ge(001) specimen was n-type, lightly phosphorus doped with a resistivity in the order of 2200 Ω cm. The Ge specimen was degassed for 8 h at 873 K before being cleaned by Ar^+ bombardment followed by direct heating to 1100 K while maintaining the system pressure below

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5×10^{-10} mbar. All temperatures above 600 K were monitored by optical pyrometry while lower temperatures were obtained by extrapolation of the higher temperature readings. After cleaning, low energy electron diffraction (LEED) revealed a two domain 2 × 1 LEED pattern indicative of a Ge dimerized surface. Silicon deposition on the Ge(001)-2 × 1 surface was achieved by electron beam evaporation using an Omicron EFM3 evaporator. The Ge substrate was held at 623 K during the Si evaporation in order to create a Si-2 × 1 dimer overlayer. The Si overlayer thickness was determined using monochromated x-ray photoemission (XPS) by comparing the intensities of the Si 2p and Ge 2p core levels. The Si submonolayer coverage was estimated to be ∼0.5 ML. The surface cleanliness was confirmed by monitoring the region of the XPS spectrum where the C and O 1s core levels appear. Once Si evaporation was achieved, even at submonolayer coverages, the 2 × 1 reconstruction remained for extremely long periods indicating that the newly formed Si/Ge(001)-2 × 1 surface remained passivated. The Si KLV Auger spectra were excited using Ti x-rays. The KLV spectra of Si are weak, ∼50 times less intense than the $KL_{2,3}L_{2,3}$:$^1D_2$ transition [11]. The accumulation period for achieving good signal to noise Si KLV spectra was of the order of 12 h which was easily obtainable with the good Si/Ge(001)-2 × 1 surface passivation.

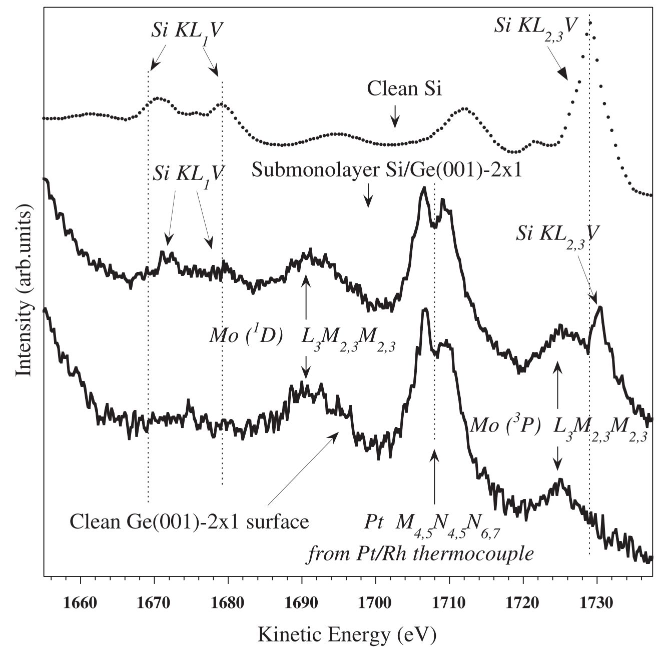

Figure 1. Shows a comparison of the Si KL_1V and $KL_{2,3}V$ Auger spectra of pure Si [12] (top curve) with the spectra of a submonolayer Si/Ge(001)-2 × 1 interface (middle curve). The spectrum of the Ge(001) clean 2 × 1 substrate region prior to Si deposition is shown in the bottom curve.

3. Results

The region of the electron spectrum in which the Si KLV transitions appear is shown for pure Si [12], the Si/Ge(001)-2 × 1 submonolayer interface and also for the initial clean Ge(100)-2 × 1 surface in figure 1.

The spectrum observed from the Ge(001)-2 × 1 substrate includes contributions from the Pt $M_{4,5}N_{4,5}N_{6,7}$ transitions of the Pt/Rh thermocouple and the $L_3M_{2,3}M_{2,3}$:^1D and ^3P transitions of the Mo clips that hold the specimen in place. Figure 1 shows that the Pt and Mo features do not overlap with the Si KL_1V transition observed following deposition of Si on Ge but that the Mo $L_3M_{2,3}M_{2,3}$:^3P transition overlaps with the low kinetic energy region of the Si $KL_{2,3}V$ transition. The Auger profile of the $KL_{2,3}V$ transitions of Si deposited on Ge was deduced by subtracting the lineshape of the Mo $L_3M_{2,3}M_{2,3}$:^3P transitions from the spectrum observed from the submonolayer coverage Si/Ge(001)-2 × 1 interface and is shown in figure 2(a) together with the experimental results of Fowles *et al* [12]. In figure 2(a) the $KL_{2,3}V$ profile of the Si/Ge(001)-2 × 1 submonolayer coverage interface has been shifted in kinetic energy by −1.6 eV to make it easier to compare the spectral profiles.

Figure 2(b) shows the profiles observed for the Si KL_1V transitions from the submonolayer Si/Ge(001)-2 × 1 interface and the experimental results for pure clean Si given by Fowles *et al* [12]. The Si KL_1V profile in figure 2(b) of the submonolayer coverage Si/Ge(001)-2 × 1 surface has also been shifted in kinetic energy by −1.6 eV to make it easier to compare the spectral profiles.

4. Discussion

The spectral profiles of the Auger transitions of Si that involve valence levels have been investigated by a number of groups with the aim of probing the influence of core-hole screening, the local atomic charge, the local valence DOS, the band structure, matrix element effects and the effects of electron correlation [12–20]. The subject has been reviewed [21].

In agreement with results obtained from theoretical calculations Fowles *et al* [12] identified three peaks in their high resolution measurements of the Si KLV profiles. The most bound and least bound of the three peaks arise from the local s and p valence DOS respectively and the middle peak has contributions from both the local s and p valence DOS. These authors analyzed the Si KLV lineshapes in terms of an empirical expression deduced from the final state rule [14, 21–25].

$$A_{\mathrm{ccv}}(E) = M^2_{\mathrm{ccs}} D_{\mathrm{s}}(E) + M^2_{\mathrm{ccp}} D_{\mathrm{p}}(E) \quad (1)$$

where the M_{ccl} terms are the energy-independent matrix elements for the transitions which produce final state holes with angular momentum l. The $D_l(E)$ are the angular momentum decomposed screened DOS in the presence of a core hole which are normalized to unit area. Equation (1) is based on two important assumptions the first of which is that the final state rule applies to Auger transitions so that the intensity of valence contributions of orbital character l to the Auger profile is determined by their contribution to the local valence configuration in the initial state and their shape by the local DOS of l character in the final state. By the final state

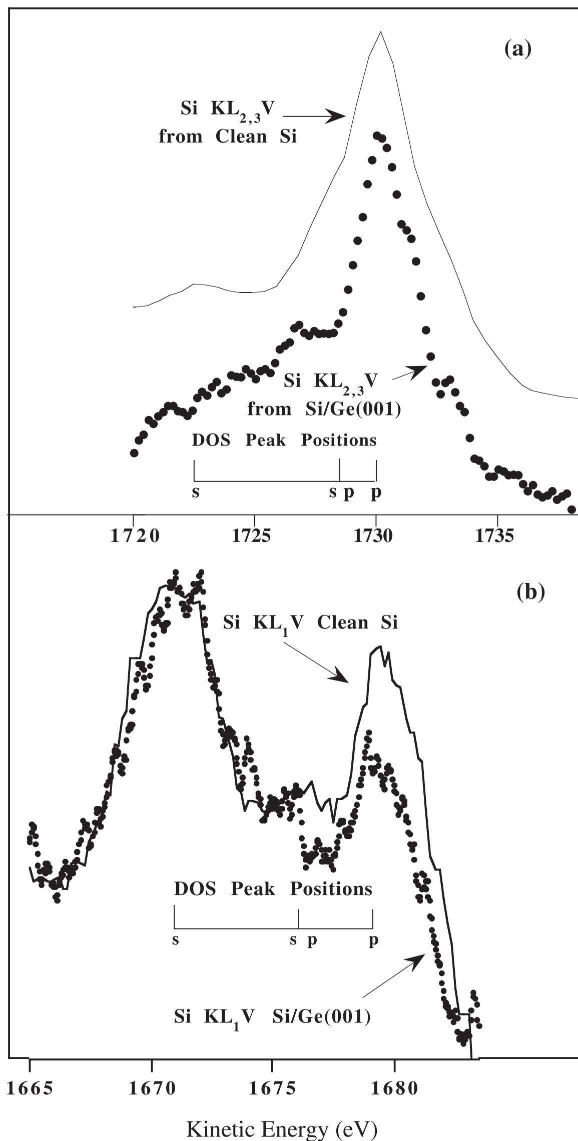

Figure 2. (a) The top curve (solid-line) shows the $KL_{2,3}V$ results obtained for pure Si [12] and the bottom curve (dots) show the submonolayer Si/Ge(001)-2 × 1 interface spectra after subtracting the contribution to the spectrum from the Mo clips. (b) The top curve (solid-line) shows the experimental results for the Si KL_1V spectrum of pure Si obtained by Fowles *et al* [12]. The bottom curve (dots) are the results obtained from the submonolayer Si/Ge(001)-2 × 1 interface. The Si KLV spectra observed from the Si/Ge(001)-2 × 1 interface in both (a) and (b) have been shifted by 1.6 eV to lower kinetic energy in order to make it easier to compare the profiles. The DOS positions of the s, sp and p peaks are shown for clarity in both figures.

rule both the spectral profiles and the relative intensity of the s and p valence contributions to the Si KLV profiles will be given by the local configuration in a core-ionized state. The second assumption underlying equation (1) is that the Auger matrix elements are independent of the energy of the valence states. This latter assumption has been investigated for the KLV transitions of Mg [26] where the matrix elements were found to have a smoothly varying energy dependence.

Fowles *et al* [12] were primarily concerned with assessing whether the Si KLV transitions could provide insight into electron correlations in Si. Studies of narrow d band metals have shown that CCV and CVV Auger profiles are determined by the relationship between the on-site correlation energy, U, and the single electron bandwidth, W [27–31]. When $U > W$ the two-hole final states created in Auger processes give rise to a quasi-atomic spectral profile in which bound states are split off from the d band DOS. These localized two-hole states have a rich multiplet structure arising from the coupling of the spin and orbital angular momenta of the individual electrons and described by the total L, S and J quantum numbers of the final states. The correlation energy is primarily an on-site quantity but off-site interactions can also influence Auger profiles as discussed for the Si KVV transitions by Verdozzi *et al* [32]. This subject has been reviewed [33].

The band width, W, of Si is considerably larger than for the d band metals and one might expect that correlation effects on the profile of the KLV transitions would be small. However by comparing the experimental results with calculated Auger profiles deduced from theoretical results for the local screened $D_s(E)$ and $D_p(E)$ on a core-ionized site obtained firstly from the linear-muffin-tin-orbital-atomic-spheres approximation (LMTO-ASA) and secondly from a modification of the LMTO-ASA results using the on-site Cini–Sawatzky treatment of electron correlation Fowles *et al* [12] concluded that correlation effects do influence the profiles of the Si KLV transitions and reasonable, though not perfect, agreement with experiment could be obtained using both approaches. They deduced values for the on-site correlations for s and p valence states, U_s and U_p, of 4.0 eV and 2.3 eV respectively which are in good agreement with those deduced by Ramaker *et al* [17]. Chang and Shirley [20] have compared the high resolution Si KLV spectra of Fowles *et al* [12] with first principles calculations that take into account core-hole screening, final state interaction effects and the angular dependence of the local DOS and which are consistent with the final state rule. They achieve a similar degree of agreement with experiment to that obtained by Fowles *et al* [12] using the semi-empirical approach based on equation (1). The main conclusions from this previous work on the KLV Auger profiles of Si are that the profiles are dominated by the contributions from the screened core hole $D_s(E)$ and $D_p(E)$ DOS and that correlation effects have an important influence on the spectral profiles. However the effect of electron correlation is much weaker than observed for the d band metals and it does not lead to the formation of bound states split off from the local valence band DOS.

The clearest evidence that the $D_s(E)$ and $D_p(E)$ DOS dominate the Si KLV spectra comes from the different relative contributions that they make to the KL_1V and $KL_{2,3}V$ profiles. The dependence of the M_{ccs} and M_{ccp} matrix elements on the angular momenta of the core holes, the valence holes and the ejected electrons involved in the Auger process results in the KL_1V having roughly equal contributions from $D_s(E)$ and $D_p(E)$ (figure 2(b)) while the $KL_{2,3}V$ is dominated by $D_p(E)$ and shows only a weak contribution from $D_s(E)$ (figure 2(a)). Studies of KLV processes in simple metals and their alloys [34–40] show that the local s and p DOS respond differently to the presence of a core hole. The s DOS is

particularly sensitive to the difference in charge between the core-ionised site and local sites that do not have a core hole. As this difference increases the s DOS is distorted so as to increase the intensity towards the bottom of the band. In simple metals the p DOS is less distorted by the presence of a core hole but its intensity increases as the difference in charge between the core-ionized sites and a local site without a core hole increases. The electronic structure calculations of [12] and [20] lead us to expect that as in the simple metals and their alloys the screening of the final L shell core hole in Si is largely accomplished by pulling the local s DOS towards the bottom of the band whereas the shape of the local p DOS is less effected by the L shell core hole.

The only study we know of in which the Si KLV Auger profiles are compared in different Si environments is our recent study of polydimethylsiloxane (PDMS) by Haines *et al* [41]. In PDMS both the KL_1V and $KL_{2,3}V$ profiles show a single feature and when compared to the spectra of pure Si show that the local p DOS is shifted to higher binding energies. This change is to be expected since in the ground state of PDMS the Si sites have oxygen and CH_3 neighbors and it is expected that there will be some charge transfer from the Si to the oxygen. This charge transfer might be expected to be from the Si p DOS thus reducing its contribution to the KLV spectra. The remaining charge will then be pulled to higher binding energy in order to screen the core-ionized site. The PDMS study shows that an oxygen plasma treatment causes a small shift in the local d DOS of Si to lower binding energy while the exposure of this surface to glycine produces a similar shift of the local p DOS to higher binding energies. The PDMS study supports our view that the Si KLV spectra can provide insight into charge distributions at interfaces.

We turn now to an analysis of the Si/Ge(001)-2 × 1 interface. As anticipated the photoelectron spectra of the valence band do not provide any insight into the electronic structure of the interface since the spectra are dominated by contributions from the bulk DOS of Ge and, in these experiments, from the spectra arising from the Pt/Rh thermocouple and the Mo clips holding the specimen in place. However the Si KLV Auger profiles do provide insight into the electronic structure of the interface particularly when analyzed in the light of the previous discussion. As indicated above the relative intensity of the $D_s(E)$ and $D_p(E)$ contributions to the spectral profiles are roughly equal for the $KL_{2,3}V$ transitions but are in the ratio ∼1:5 for the KL_1V transitions. Since the profiles of the Si KL_1V and $KL_{2,3}V$ transitions show such a different dependence on $D_s(E)$ and $D_p(E)$ a comparison of their relative intensities and lineshapes with those of pure Si provide insight in the difference in the local DOS around a Si atom in Si and a Si atom at the Si/G(100)-2 × 1 surface. We begin with an estimate of the relative intensity of the KL_1V:$KL_{2,3}V$ transitions. In pure Si the results of Fowles *et al* [12], after allowing for the background of scattered electrons, give a value of

$$I(KL_{2,3}V)/I(KL_1V) = 6.3 \pm 0.1.$$

The error quoted on this ratio is probably a significant underestimate due to the difficulty of accounting for systematic errors arising from uncertainly in allowing for the background of scattered electrons. Obtaining an estimate for this ratio for the Si/Ge(001)-2 × 1 interface is further complicated by the overlap of the Si $KL_{2,3}V$ profile with the Mo $L_3M_{2,3}M_{2,3}{:}^3P$ excited from the sample clips (figure 1). By comparing the spectral region of the Si $KL_{2,3}V$ spectrum obtained from the Si/Ge(001)-2 × 1 interface and the clean Ge(001)-2 × 1 surface and then by subtracting the Mo $L_3M_{2,3}M_{2,3}{:}^3P$ profile from the spectrum of the Si/Ge(001)-2 × 1 interface, we obtain the result

$$I(KL_{2,3}V)/I(KL_1V) = 2.3 \pm 0.3$$

where the increased error reflects the difficulty of allowing for the Mo $L_3M_{2,3}M_{2,3}{:}^3P$ profile but does not include the contribution from systematic uncertainty in estimating the contribution from the background of scattered electrons. Given the dominance of the $D_p(E)$ DOS in the $KL_{2,3}V$ these results suggest that the intensity of the local p DOS is significantly reduced in intensity relative to the s DOS for Si atoms at the Si/Ge(001)-2 × 1 interface.

We now consider the detailed spectral profile of the Si $KL_{2,3}V$ transitions which are shown in figure 2(a) together with the experimental results for pure Si. It is not possible to be sure of the profile obtained from the interface for kinetic energies lower than 1727 eV due to the sensitivity of this region to the subtraction of the Mo peak. However it is clear from the spectrum that the contribution from $D_p(E)$, which occurs to high kinetic energy, is narrower than in pure Si. The narrowing reveals two shoulders on the high kinetic energy side of the peak at ∼1731.2 and 1733.0 eV. These features can just be discerned but are very much weaker in the pure Si $KL_{2,3}V$ profile.

Figure 2(b) shows a comparison of the spectral profile of the Si KL_1V transitions observed from the Si/Ge(001)-2 × 1 interface with the experimental results for pure Si. This comparison shows that $D_p(E)$ makes a significantly weaker and narrower contribution to the spectrum observed from the Si/Ge(001)-2 × 1 interface than it does in either the spectrum observed from Si or given by the theoretical results [12].

The narrowing and reduction in intensity of the contribution of the p DOS to the KLV profiles obtained from the interface together with the results obtained from the comparison of the $I(KL_{2,3}V)/I(KL_1V)$ intensity ratios of the interface and pure Si leads to the conclusion that the p DOS is significantly reduced on a core-ionized Si site at the interface from its value at a core-ionized site in pure Si.

It is clear from the above that the screening of core holes on Si sites at the Si/Ge(001)-2 × 1 interface is significantly different from the screening of core holes in pure Si. In particularly the contribution from the p DOS is significantly reduced. An examination of the results of theoretical calculations [21] indicates that while an increase in the on-site electron correlation, U_P, for p states could go some way towards explaining the changes that are observed in the $KL_{2,3}V$ spectral profiles this is unlikely to be the major factor since while increasing U_P will redistribute the local $D_p(E)$ to high binding energy the total intensity of the $D_p(E)$ contribution to the KLV spectral profiles will be preserved. Consequently this

could not explain the large reduction in the intensity of ratio, $I(\mathrm{KL}_{2,3}\mathrm{V})/I(\mathrm{KL}_1\mathrm{V})$, which indicates that the total intensity of the $D_\mathrm{p}(E)$ contribution is reduced at the interface.

The most plausible explanation for the reduced intensity of the $D_\mathrm{p}(E)$ core-hole screening charge at the interface is that it reflects changes in the local DOS in the ground state at the interface compared to pure Si. This suggests a very strong transfer of p charge from the Si atoms at the interface to the Ge sites. This is a similar, but much weaker, effect to that observed in PDMS. We conclude that in the ground state the electronic structure of the interface is characterized by a transfer of charge from the Si valence p DOS states to the Ge sites and that in consequence the local p DOS of states on a Si site is narrower and weaker than in pure Si.

The conclusion that there are substantial charge transfers at the Si/Ge(001)-2 × 1 interface is consistent with the results of Jenkins and Srivastava [3]. These authors modeled the structure and energetics of segregated and non-segregated Si/Ge(001)-2 × 1 interfaces using *ab initio* pseudopotential density functional calculations. They concluded that the segregated Ge terminated surface would be more stable than the Si terminated structure by some 0.38 eV per dimer.

One final point to note is that while the Si KLV profiles provide direct information on the screening of core-ionized states and indirect information on the DOS at the interface, by the equivalent cores approximation the $D_\mathrm{s}(E)$ and $D_\mathrm{p}(E)$ DOS that we observe will be very similar to those of P impurities at this interface.

5. Conclusion

An analysis of the differences in the Si KLV Auger profiles between pure Si and the Si/Ge(001)-2 × 1 interface indicate that the electronic structure of the interface is characterized by a reduction in the local p DOS on the Si sites and a transfer of p valence charge from Si to Ge. As a result the balance of the screening of core-ionized Si sites at the interface is significantly shifted towards s screening compared to the situation in pure Si. It is possible that there is an increase in the on-site electron correlation energy, U_P, on Si sites at the interface compared to pure Si though this is unlikely to make a major contribution to the changes observed in the Si KLV spectra.

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