Soft-x-ray photoemission study of chemisorption and Fermi-level pinning at the Cs/GaAs(110) and K/GaAs(110) interfaces

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The room-temperature adsorption of Cs on n-type GaAs(110) has been studied with use of core-level photoelectron spectroscopy. The coverage-dependent splitting of the Cs 4d core level into two sets of doublets indicate site-dependent adsorption for submonolayer coverages up to about 0.5 monolayer (ML). The broadening of this core level close to the saturation coverage is consistent with the growth of an out of registry monolayer as suggested by low-energy electron diffraction (LEED) data. Analysis of the substrate core levels indicate the formation of a laterally uniform overlayer and lack of chemical reaction. The Schottky barrier of 0.7 eV obtained from the low-coverage band bending is similar to the values for many other metals with much larger work function (Al, Ni, or Ti). We report also data on the K overlayers. They indicate a similar value of band bending and presence of a chemical reaction at the K/GaAs interface. The band bending results for Cs and K indicate that Schottky barrier for GaAs interfaces do not depend on the metal work function in a very broad range of the work-function values.

I. INTRODUCTION

In this work we report a core-level photoemission spectroscopic (PES) study of the chemisorption and the chemisorption-induced band bending at the Cs/GaAs(110) and K/GaAs(110) interfaces. The Fermi level pinning at these interfaces is of interest because of extremely small electronegativities and work functions of alkali metals. This provides a useful test of the Schottky-barrier models. Indeed it seems that understanding the Cs alkali-metal data is a challenge to the Schottky-barrier models which have to explain the bend bending and the simultaneous large decrease of the GaAs work function induced by overlayer (3.8 eV). The theoretical calculation of Zur et al.[1] based on the defect model of Spicer et al.[2] and the use of jellium to model a metallic overlayer fails to explain why Cs or any alkali metal could pin the Fermi level in the mid gap. For a very small value of the metal work function, the Fermi level cannot be lowered enough to pin at the defect level independent of their density. Spicer et al. pointed out this problem and proposed an alternative atomic model for Cs interfaces, which incorporates a large atomic dipole also necessary to explain the substrate work-function reduction.[3] The important assumption of the Zur et al. work that the adatoms (submonolayer coverages) do not contribute any significant amount of charge, is questionable for the Cs overlayers. Recently, the problem of the bend bending and work-function lowering has been addressed by Monch from the point of view of metal in-

duced virtual gap states.[4] In this model the decrease of the work function is attributed to the charge transfer from electropositive Cs to the virtual gap states of GaAs. The charge transfer also causes the movement of the Fermi level above the charge-neutrality level calculated by Tersoff at 0.5 eV above the valence-band maximum (VBM).[5] It is assumed that without charge transfer the Fermi level should be pinned at the charge neutrality level.

Due to the renewed interest in alkali-metal interfaces we decided to perform a new core-level PES study of the Cs/GaAs interface to fill up certain gaps in the older literature. For example, we were unable to find any reliable data on the bend bending for the n-type substrates. The early work of Gregory and Spicer[6] to which most of the authors refer in this context provides a reliable information on the band banding for the p-type substrates only. The authors concluded from the valence band PES data that the surface Fermi level for p-type samples moves to about 0.6 eV above VBM (although for some samples even larger band bending was observed). This result agrees with later determinations. It also agrees well with photovoltaic measurements of Uebbing and Bell performed on the thick layers of Cs condensed on the p-GaAs(110) surface at liquid nitrogen temperature.[7] These authors reported a barrier height of 0.63±0.03 eV. A large interest in the cesiated p-GaAs stems from the possibility of obtaining negative electron affinity (NEA) condition which has some unique device applications. The measurements of the n-type GaAs are sparse, con-

tradictory and often unreliable. For example Gregory's experiment was performed during the time when most groups failed to obtain unpinned n-type GaAs(110) surfaces. The reason for this is not clear but seems to be related to the lower quality of available crystals rather than to problems with the relatively easy technique of cleaving. Gregory and Spicer[6] found that the Fermi level located 0.5 eV below the conduction-band minimum (CBM) on the cleaved surfaces was not affected by the Cs depositions and consequently concluded that the barrier height on n-type GaAs is only 0.5 eV. This value is suspect because the origin and the density of states responsible for the initial Fermi-level pinning is unknown.

This work emphasizes the Fermi-level pinning at the Cs/GaAs interface. Consideration will be also given to other aspects of Cs chemisorption. Some of these issues were studied earlier by many workers using a variety of techniques.[8-14] These and our results show that in many respects the properties of this interface are unique (some analogies to Sb chemisorption will also be considered). This is a clear-cut case of a nonreactive and abrupt GaAs interface for which the possibility of island formation is precluded by the low heat of adsorption of Cs on Cs.

II. EXPERIMENT

The experiments were performed on the Mark II grasshopper monochromator beam line at the Synchrotron Radiation Center of the University of Wisconsin–Madison. The photoemission spectra were taken in a standard ultrahigh-vacuum (UHV) chamber (base pressure 5×10^{-11} Torr) equipped with a double-pass cylindrical mirror analyzer. The Ga $3d$, As $3d$, and Cs $4d$ levels were monitored for cleaved GaAs(110) and Cs-covered surfaces. The depositions of Cs and K were done from SAES Getters (Italy) chromate sources. The Cs source was carefully calibrated using Cs $4d$ core level intensity, which exhibits saturation for certain coverage which we define as 1 monolayer (ML). It is established that at room and higher temperatures one cannot obtain stable overlayers above this saturation coverage. Due to the large size of Cs atoms the saturation coverage corresponds to 0.55 of a monolayer according to the traditional definition in terms of the GaAs surface density (1 ML $= 8.85 \times 10^{14}$ atoms cm^{-2}). Throughout this paper the saturation coverage, in agreement with the Cs literature, will be referred to as a monolayer. We also performed a preliminary study for the K/(n-type GaAs) interface. In the case of K the calibration of the source was not certain, although we estimate, from the substrate core-level attenuation, that highest exposures could be in excess of a monolayer. (The K core level overlaps with the Ga $3d$ core level and therefore cannot be used to monitor coverage.) Because of the calibration uncertainty only the time of evaporation of K source operated at a constant current of 5.4 A (above the warm-up time of 50 sec) will be given. For both Cs and K sources the alkali coverage was proportional to the evaporation time and the pressure during evaporations was kept below 2×10^{-10} Torr.

III. RESULTS

Figures 1 and 2 show the Ga $3d$ and As $3d$ spectra for the Cs/[n-type GaAs (110)] interface. Both core levels simultaneously shift to higher kinetic energy as the bands bend upward with Cs coverage. The lack of the additional chemically shifted components in the core levels is taken as evidence of no chemical reaction between the Cs and GaAs. This allows a straightforward determination of the band bending from the spectra. The results plotted in Fig. 3 show that the Fermi position stabilizes at 0.7 eV below the conduction-band minimum (CBM) for about 0.4 ML. This pinning energy is within the experimental error (± 0.05 eV) identical to that obtained from the photoemission data for the model Al/GaAs interface.

The identical intensity attenuation of the Ga $3d$ and As $3d$ core levels (not shown; spectra for the substrate core levels are normalized to the same height to better visualize the line-shape changes) and a lack of chemical reaction ascertains a laminar growth and abruptness of the interface.

Valuable information on the Cs chemisorption is provided by the Cs $4d$ core-level spectra presented in Fig. 4. For coverages up to 0.45 ML these spectra contain two components correlated with the different adsorption sites. At the highest coverage the spectrum broadens and a Doniach-Sunjic line shape[15] is observed. This result indicates metallization of the overlayer. For all spectra corresponding to coverages up to 0.45 ML we performed a curve fitting of the Cs $4d$ with two doublets. An example of such a curve decomposition of the 0.04 ML spectrum
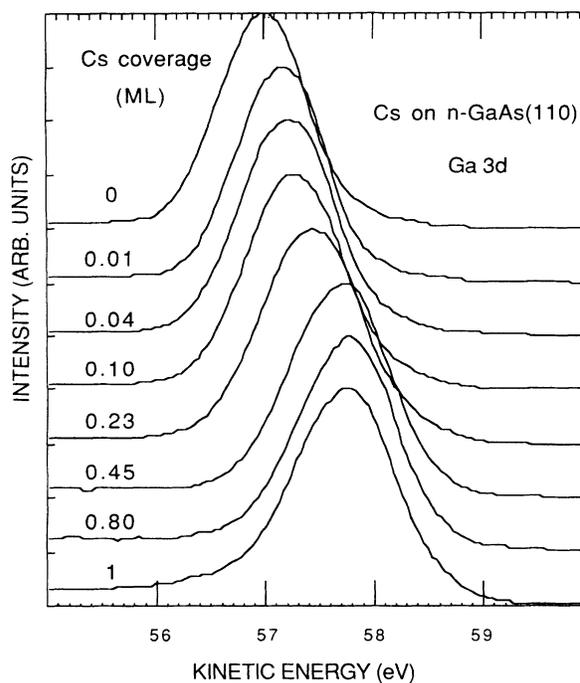

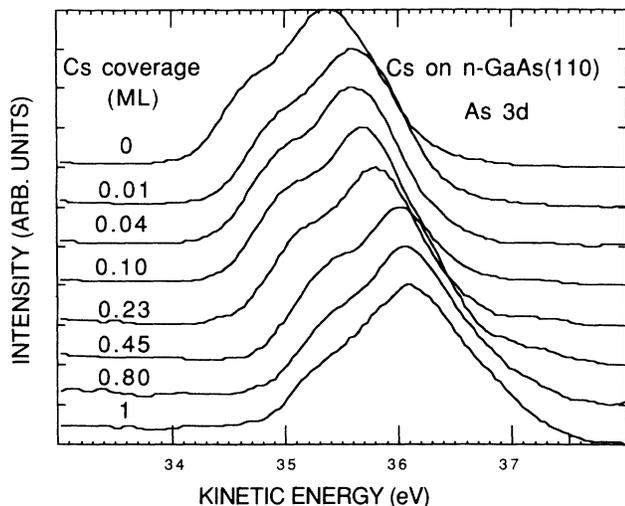FIG. 1. Ga $3d$ core-level spectra taken at 80 eV for thin Cs overlayers on n-type GaAs(110).

FIG. 2. As 3d-core-level spectra taken at 80 eV for thin Cs overlayers on n-type GaAs(110).

FIG. 4. Changes in the Cs 4d core level for Cs covered on GaAs(110) (photon energy of 120 eV).

for 2.3-eV spin-orbit splitting, 0.7-eV Gaussian width (taken as the overall instrumental resolution), and near statistical branching ratio (1.4) in each doublet, is shown in Fig. 5. These parameters were kept constant during the fitting. The energy difference between the two doublets decreases monotonically from 0.78 eV for 0.01 ML to 0.48 eV for 0.45 ML (see Fig. 6). The intensity ratio of the components is close to unity (the ratio depends critically on the fitting parameters and is less reliably determined), and the Lorentzian part of the line width increases slightly from 0.30 to 0.35 eV. A formal, but less satisfactory, fit with two doublets is possible also for 0.8 ML but a dramatic increase in the Lorentzian part of the line width (over 50%) obtained from the fit indicates different physical behavior [possibility of additional un-
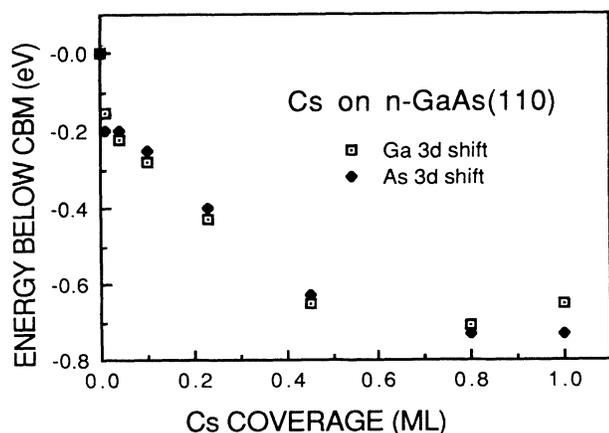
resolved component(s) can not be excluded]. We believe that, because the system is not well represented by the imposed model, the increase of the Cs 4d splitting for this coverage (not shown) is not physical. This conclusion is consistent with changes in the line shape seen in the raw data.

The Cs/GaAs interface with 1 ML Cs coverage was also exposed to the pure molecular nitrogen to study the effect of these highly electronegative atoms on the band bending. We observed that the highest studied nitrogen exposure of 4000 langmuirs (1 L $\equiv 10^{-6}$ Torr sec) causes a shift of both Ga 3d and As 3d core levels by 0.2 eV toward the conduction band. Nitrogen exposures did not

FIG. 3. Fermi-level movement at the Cs/GaAs interface as determined from the shifts of the As 3d and Ga 3d-core-level spectra.

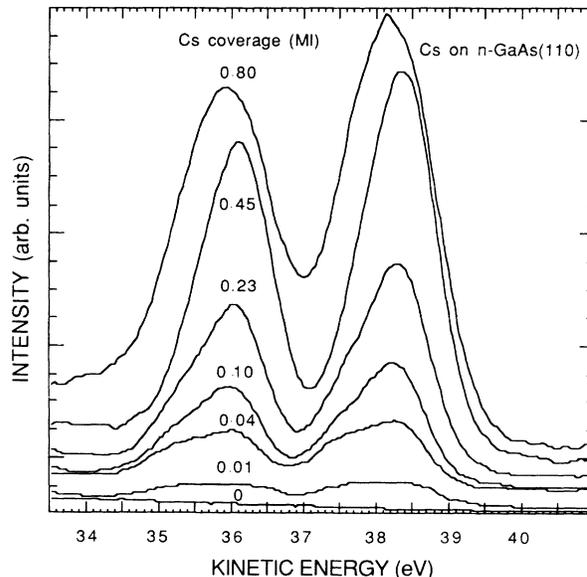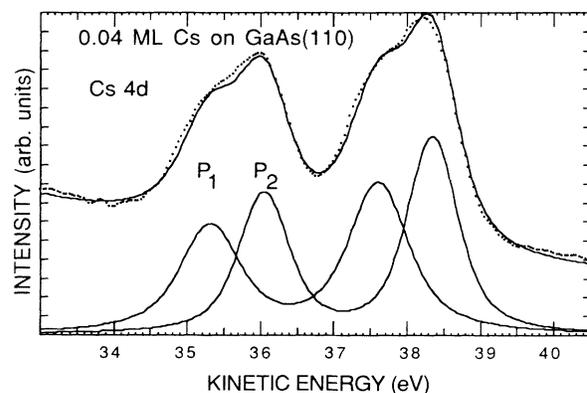FIG. 5. Curve fitting of the Cs 4d spectrum for 0.04 ML of Cs with two doublets corresponding to different adsorption sites. The dots represent the data and the upper solid line is the sum of the components P1 and P2.
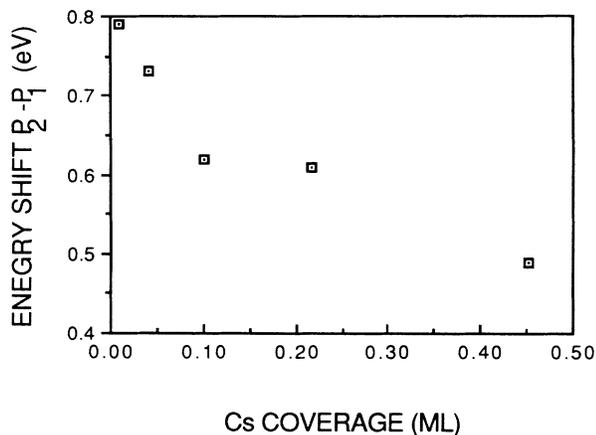
FIG. 6. Change of the splitting between $P1$ and $P2$ components of the Cs $4d$ level for increasing Cs coverage (see Fig. 5) using data presented in Fig. 4.

cause any noticeable change of the core-level line shapes nor produce new chemically shifted components. This indicates that N does not react with the Cs/GaAs interface. From earlier studies it is known that Cs may increase the uptake of oxygen[16] and causes a decrease of the band bending for n-type GaAs and an increase for the p-type doping. The increase of (downward) bend bending in conjunction with induced by oxygen further decrease of the bend bending (dipole part) may produce a condition of negative electron affinity in which vacuum level of the GaAs surface is lower than the CBM in the bulk.

We also studied the K/GaAs interface. Due to the uncertainty of the K calibration these results should be treated as preliminary. However, even without the precise knowledge of the coverage we can establish facts which are of key importance for our purpose. First, the data show that the final band bending at this interface is at least equal to that in the Cs/GaAs case. Figure 7 shows the bend bending from the Ga $3d$ and As $3d$ core levels as a function of the time the interface is exposed to the K source. To establish the band bending a curve
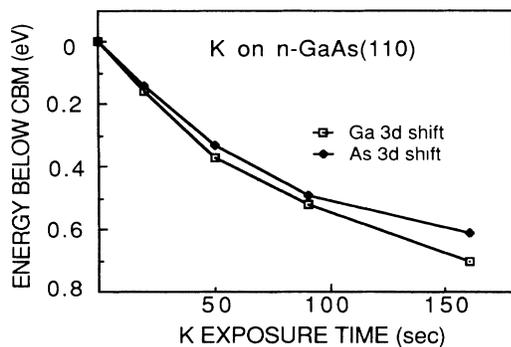
fitting was performed to account for the chemical reaction and possible overlapping of the very weak K $3p$ core level with the Ga $3d$. The presence of some chemical reaction which distinguishes this system from described above Cs interface can be seen in Fig. 8, which shows the As $3d$ spectra. The example of curve fitting with two doublets (of statistical branching ratio and 0.69-eV spin-orbit splitting) for the highest K exposure of more than a ML is shown in Fig. 9. The high kinetic energy component, chemically shifted by 0.75 eV, dominates the spectrum.

To study the influence of the electronegative species on the bend bending we exposed the interface to molecular oxygen. As for N deposited on the Cs/GaAs interface we observe the Fermi level movement toward the conduction band minimum (reduction of the band bending). This shift for the exposure of 100 L amounted to 0.4 eV, i.e., twice the value of the N/Cs/GaAs system. The presence of the K layer causes a dramatic increase of the oxidation rate. This is shown in Fig. 10 which compares the As $3d$ spectrum from the K/GaAs interface and the same interface exposed to 100 L of oxygen. The new low kinetic energy peak provides a clear indication of oxidation. To obtain a similar oxidation rate on clean surfaces one needs at least five orders of magnitude more oxygen (the case of excited oxygen). The increased oxidation rate is seen also for lower exposures (32 L). However, for 1 L, when the effect is not noticeable, we observe some reduction of the band bending. We conclude that both N and O atoms sticking to the alkali-metal interfaces reduce the band bending on n-type GaAs. This reduction is independent of the presence or absence of a chemical reaction between GaAs and these atoms which can be enhanced (for example, oxygen) by the presence of alkali metals.

IV. DISCUSSION

A. Chemisorption

The Cs $4d$ data (Fig. 4) provide a great deal of information on the chemisorption. We distinguish two Cs coverage ranges with distinctly different physical properties.
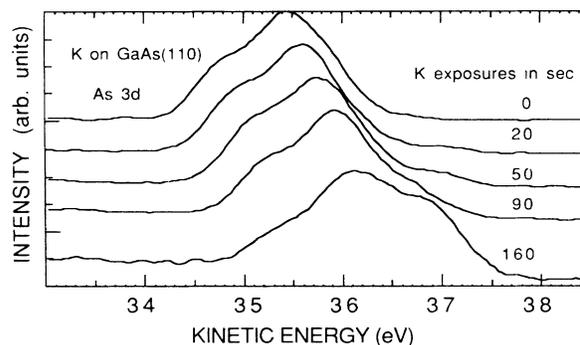

FIG. 7. Fermi-level movement at the K/GaAs interface as a function time of K deposition.

FIG. 8. As $3d$ core-level spectra at 80 eV from the K/GaAs(110) interface.
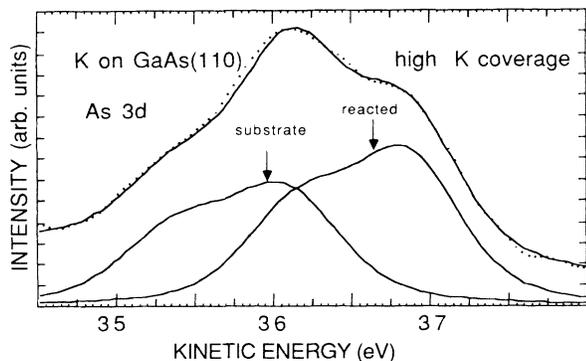
FIG. 9. Example of curve fitting of the As $3d$ spectrum with around 1 ML coverage indicating presence of a reacted peak shifted by 0.75 eV.

Up to about 0.5 ML we observe a characteristic splitting of the Cs $4d$ indicative of adsorption at two different adsorption sites. The broadening at higher coverages is consistent with a random absorption position or growth of an out of registry monolayer. It is interesting to note that the general picture of the Cs chemisorption obtained from these data is consistent with some previous studies. There are, however, some differences in detail which will be pointed out below. Several authors have studied the absorption of Cs on GaAs(110) using LEED, Auger-electron spectroscopy (AES), and other techniques.[8–14] In addition, changes in the photoelectron yield and work function for the increasing Cs dosage have been well documented.[8,9,11] References 8, 9, 11, and 14, which report studies on the (110) studies are of particular interest for our discussion. However, work on other surfaces also contributes to the understanding of the Cs chemisorption.
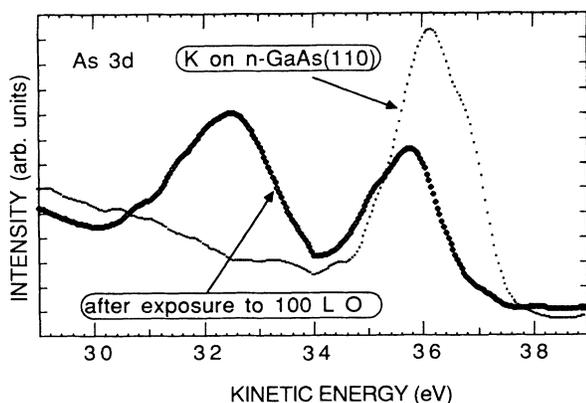
At room temperature LEED shows mainly one

FIG. 10. Enhanced reaction of the GaAs with O at the K/GaAs interface evidenced from changes in the As $3d$ spectra. Notice that bulk As $3d$ at higher kinetic energy indicates reduction of the band bending.

pattern—$c(4\times4)$,[8] although some indication that other reconstructions may be present. The $c(4\times4)$ pattern is observed between 0.5 and 1 ML.[8,9] It is also established that close to 0.5 ML the work function passes through a minimum which corresponds to the maximum of the photoemissive yield and the negative electron affinity for p-type GaAs. The thermal desorption experiments indicate that below 0.5 ML Cs is particularly strongly bound. Derrien and Arnaud d'Avitaya suggested that at low coverages Cs atoms are located at well defined remote adsorption sites.[9] The same conclusion has been reached by Clemens *et al.*[11] on the basis of the work-function studies. They observed several breaks in work-function dependence on the coverage and correlated these with completion of certain adsorption patterns. It is suggested that the dipolar repulsion puts Cs atoms in remote positions on the surface. This maximizes the reduction of the work function. As the Cs coverages increases the shrinking Cs-Cs distance causes some depolarization and related to this slight increase of the work function. Close to the saturation coverage, the overlayer is more loosely bound. There is a consensus that the $c(4\times4)$ reconstruction which is completed at 1 ML corresponds to an out of registry superstructure in which the Cs overlayer is randomly and nondirectionally bonded to the substrate. The model proposed[8,9] for the $c(4\times4)$ pattern is characterized by a 14% compression of the Cs-Cs distance in one of the directions (4.6 Å relative to 5.2 Å in metallic Cs). Most of the Cs atoms are no longer localized on the adsorption sites. The substrate and the overlayer atoms are bonded to each other through a metallic bond.[17] Beyond the saturation coverage the $c(4\times4)$ superstructure fades away and the extra Cs atoms at room temperature are very weakly bonded to the substrate[8,9,10] and in nonequilibrium conditions (UHV with no continuous incoming Cs flux) desorb from the overcesiated surface. Studies of slightly annealed surfaces indicated the presence of other surface reconstructions in the submonolayer coverage range. In particular, all authors report the presence of a $c(6\times2)$ reconstruction. There are some indications that this reconstruction may be present on nonannealed surfaces[8,9,14] but is substantially enhanced by an anneal of about 250 °C. The most complete LEED study has been reported by Derrien and Arnaud d'Avitaya[9] who identified another low-coverage reconstruction $[p(3\times2^*)]$. Models for LEED data put the Cs atoms in voids in the [110] direction. There are two nonequivalent sites on the GaAs in which the chemisorption is most likely. These are shown schematically on Fig. 11. Both Derrien and Arnaud d'Avitaya[9] and Clemens *et al.*[11] favor adsorption on one site (no. 2 in Fig. 11) which is closest to the empty Ga dangling bond. The splitting in our data seems to be inconsistent for a single adsorption site for small coverages and seems to be in better agreement with Van Bommel and Crombeen's model for the $c(2\times6)$ reconstruction which uses both adsorption sites. We, however, note that this model contains very short distances in some directions between Cs atoms which are not likely if one believes in a physical model in which dipoles repel one another and drive Cs atoms to remote sites. We also believe that the assumption of single bond
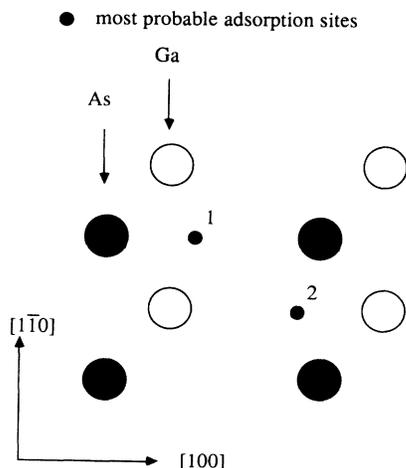
● most probable adsorption sites

FIG. 11. The schematic top view of the GaAs(110) surface with the most likely absorption sites marked as 1 and 2.

The broadening in the Cs 0.8-ML spectrum (Fig. 4) is consistent with the above outlined model of chemisorption. At this coverage the Cs is out of registry with the substrate and the Cs-substrate distances become random. In this situation one expects broadening of the overlayer core-level spectra, which is indeed observed. The decrease of the Cs-Cs distance close to 1-ML coverage causes the increase of the interaction within the overlayer. This results in the metallization of the overlayer which is evident from the skewed line shape of the Cs 4d spectra or low energy plasma loss.

The Cs and Sb interfaces have unique properties. They are abrupt on the atomic level and at the same time grow in the form of monolayers. In both cases the chemical reaction with the substrate or interdiffusion is negligible. These interfaces are ideally suitable for theoretical modeling which provides interesting results for Sb.[22] Recently Manghi et al.[17] modeled the Cs surfaces theoretically using a jellium model. It would be interesting to treat the $c(6\times2)$ reconstruction in a more realistic approach. Our results indicate that pinning of the Fermi level is complete at coverages where this superstructure occurs.

site is not necessary to explain Derrien and Arnaud d'Avitaya's[9] LEED data. Our results are clearly incompatible with the model of Clemens et al., which suggest one site adsorption for small coverages.[11]

The Cs 4d data are very similar to the results for the Sb 4d core levels at the Sb/GaAs interface reported recently by several authors[18-20] and related to the multisite adsorption. It is agreed that the Sb monolayer grows in the form of ordered zigzag chains which are parallel and in registry to the zigzag chain of the GaAs(110) surface.[21,22] In these zigzags, the Sb atoms are alternately bonded to Ga and As atoms, i.e., occupy both sites marked in Fig. 11. The Sb atoms bonded to the Ga in this chain are less strongly bound and correspond to the higher kinetic energy doublet in the Sb 4d spectrum. Although Sb and Cs atoms are chemically very different and although the type of bonding should be different, we recognize several formal similarities in the chemisorption reflected in the data. The model for the $c(6\times2)$ reconstruction proposed by Van Bommel and Combeen[8] for submonolayer Cs coverages suggests the same adsorption sites as the zigzag chain model. The difference is that, due to the large size of Cs atoms, every second atom along the [110] direction is missing and not every channel in the [110] direction is likely to be occupied. Thus, instead of zigzags, one obtains rows of Cs atoms along the [110] direction bonded to either As or Ga. The observation that both components of the Sb 4d spectra have about equal intensity indicates nearly equal occupancy of these sites. We thus suggest that this type of chemisorption is present at room temperature, although the ordering in chains may be improved after the 300 °C anneal, for which the $c(6\times2)$ pattern is seen by all workers. A similar argument was given by Schaffler et al. for the Sb interface.[18] They argued against perfectly ordered growth of the Sb at room temperature. The annealing to 330 °C was found to improve the degree of order which was monitored by the Sb 4d spectra.

B. Fermi-level pinning

In this work we established that the Cs and K overlayer deposited on the GaAs(110) surface produces bend bending of 0.7 eV. This result is consistent with the recent data of McLean et al.[23] for the Na/GaAs(110) interface. From a combined PES (for thin overlayers) and electrical study (thick overlayers), they found a barrier height of 0.69–0.72 eV from the I-V measurements which were consistent with low coverage PES data. The values reported by us and McLean et al. for the alkali metals are very similar to the bend bendings produced by some much more electronegative metals like Ti or Ni. These metals have also much larger values of the work function [4.33 (Ti) and 5 (Ni) relative to 2.13 and 2.30 for Cs and K, respectively]. The comparison of these results shows that the Schottky barrier height does not depend on the work function in a broad range of work-function values. It is also interesting to note that similar values for the Schottky barrier heights were previously established for another class of low-work-function materials—the rare-earth metals (see for example Refs. 24–26). This observation is not meant to suggest that the barrier heights for GaAs interfaces are generally independent of the metal. It is well established that the noble metals Pd or Pt produce band bendings about 0.2 eV larger than Ni or Ti. The data, however, show that there is no simple monotonic correlation between band bending and work function or electronegativity. It is intriguing to stress that this behavior of the GaAs interfaces clearly differs from what is established for Si. The barrier heights of alkali or rare-earth metals on n-type Si are 0.3 to 0.4 eV smaller than for Al.[27] The barriers for Si interfaces depend linearly on the metal work function, although, the dependence is weaker than in the Schottky model. It is also not clear to what extent the GaAs results are representative for III-V compounds. Our experiments on InP indicate a similar behavior.[28] However, Brillson et al. found good

agreement with the Schottky model for GaP interfaces.[29]

The independence of the barrier height on the metal work function for GaAs stimulated several models of Schottky barrier formation. Spicer et al. associated the Fermi-level pinning with native defects,[2] Woodall and Freeouf[30] with As inclusions, while Tersoff further developed a model in which the pinning at the semiconductor charge neutrality level results from tails of the metal induced gap states (MIGS).[5] Recently, Monch and co-workers[4,31] proposed a model which extends Tersoff's concept to the small coverage bend bending studied in photoemission experiments. This model explains the chemical trends in the barrier heights through the charge transfer between the virtual gap states (VIGS) of the complex band structure of GaAs and the adsorbate, which does not have to be metallic. This model has been applied to the Cs/GaAs interface. As already mentioned in the introduction, Spicer et al.[3] suggested an explanation why the Cs/GaAs interface could produce a rectifying barrier in the context of the defect model. The models of both Monch and Spicer et al., explain (or rely on) the work-function lowering and the unexpectedly large value of the bend bending on n-type GaAs. The experimental data presented in this work (as well as in the literature) do not provide a clear-cut distinctiction between these concepts. It is also apparent that simple versions of both models fail to explain some experimental data presented in this work. In particular in the context of Monch's model one would expect that depositing electronegative O and N on top of alkali metals should increase rather than decrease (as observed) the band bending (this is due to removal of Cs electrons from the virtual states). This should be so in particular for the N/Cs/GaAs interface where no reaction is observed. To explain these data both models probably need additional defects in the upper part of the band gap.[31]

Recently, Manghi and co-workers performed the calculations of the electronic structure of the Cs/GaAs interface using the self-consistent pseudopotential method and modeling the monolayer of Cs as a jellium slab. This seems to be the only realistic approach for this out of registry overlayer. The calculations were done for both relaxed and ideal configuration of the substrate atoms. The authors conclude that for the relaxed surface, which is found to better account for available experimental data, the dangling bond states (which are found to be responsible for pinning for unrelaxed surface) remain out of the gap after metallization but the pinning energy established by Cs-induced states is still close to the CBM. The calculations fail to account for the experimental pinning levels and the authors suggest extrinsic pinning mechanisms by defects. In this work a large accumulation of the charge was found right as the interface and related to surface dipole formation and decrease of the work function by 3.8 eV (in agreement with experiment).

V. CONCLUSIONS

We have shown that at room temperature up to about 0.5 ML coverage, Cs chemisorbs in two sites on the GaAs(110) surface. This is concluded from distinct and coverage dependent splitting of the Cs $4d$ spectra. Above this coverage the metallic overlayer is not in registry with the substrate which is indicated by the broadening of the spectra. No reaction or interdiffusion is observed. In contrast, K reacts with GaAs. However, despite different chemical behavior, both alkali metals cause a large band bending of 0.7 eV, which is comparable with band bendings produced by much more electronegative metals (example Ni).

[1] A. Zur, T. C. McGill, and D. L. Smith, Phys. Rev. B **28**, 2060 (1983).

[2] W. E. Spicer, I. Lindau, P. R. Skeath, and C. Y. Su, J. Vac. Sci. Technol. **17**, 1019 (1980).

[3] W. E. Spicer, S. Pan, D. Mo. N Newman, P. Mahowald, T. Kendelewicz, and S. Eglash, J. Vac. Sci. Technol. B **2**, 476 (1984).

[4] W. Monch, J. Vac. Sci. Technol. B **4**, 1085 (1986).

[5] J. Tersoff, Surf. Sci. **168**, 275 (1986), and references therein.

[6] P. E. Gregory and W. E. Spicer, Phys. Rev. B **12**, 2370 (1975).

[7] J. J. Uebbing and R. E. Bell, Appl. Phys. Lett. **11**, 357 (1967).

[8] A. J. Van Bommel and J. E. Crombeen, Surf. Sci. **45**, 308 (1974); **57**, 109 (1976).

[9] J. Derrien and F. Arnaud d'Avitaya, Surf. Sci. **65**, 668 (1977); J. Derrien, F. Arnaud d'Avitaya, and M. Bienfait, Solid State Commun. **20**, 557 (1976).

[10] B. Goldstein and D. Szostak, Appl. Phys. Lett. **26**, 111 (1975).

[11] H. J. Clemens, J. Von Wlenskowski, and W. Monch, Surf. Sci.

78, 648 (1978).

[12] D. Rodway, Surf. Sci. **147**, 103 (1984).

[13] T. E. Madey and J. T. Yates, J. Vac. Technol. **8**, 39 (1971).

[14] A. Y. Mityagin, V. P. Orlov, V. V. Panteleev, J. A. Khronopoulo, and N. Y. Cherevatskii, Fiz. Tverd. Tela (Leningrad) **14**, 1870 (1973) [Sov. Phys.—Sol. State **14**, 1623 (1973)].

[15] S. Doniach and M. Sunjic, J. Phys. C **3**, 285 (1970).

[16] C. Y. Su, P. W. Chye, P. Pianetta, I. Lindau, and W. E. Spicer, Surf. Sci. **86**, 894 (1979).

[17] F. Manghi, C. Calandra, C. M. Bertoni, and E. Molinari, Surf. Sci. **136**, 629 (1984).

[18] F. Schaffler, R. Ludeke, A. Taleb-Ibrahimi, G. Hughes, and D. Rieger, J. Vac. Sci. Technol. B **5**, 1048 (1987); Phys. Rev. B **36**, 1328 (1987).

[19] J. R. Myron, J. Anderson, and G. J. Lapeyre, in *Proceedings of the International Conference on Physics of Semiconductors, San Franciso 1984*, edited by D. J. Chadi and W. A. Harrison (Springer, New York, 1985), p. 133.

[20]R. Cao, K. Miyano, T. Kendelewicz, I. Landau, and W. E. Spicer (unpublished).

[21]P. Skeath, C. Y. Su, W. A. Harisson, I. Landau, and W. E. Spicer, Phys. Rev. B 27, 6246 (1983), and references therein.

[22]C. Mailhiot, C. B. Duke, and D. J. Chadi, Phys. Rev. B 31, 2213 (1985).

[23]A. B. McLean, D. A. Evans, and R. H. Williams (private communication).

[24]J. R. Waldrop, Appl. Phys. Lett. 46, 864 (1985).

[25]M. D. Williams, J. Nogami, T. Kendelewicz, R. S. List, K. A. Bertness, I. Lindau, and W. E. Spicer, Solid State Commun. 58, 15 (1986).

[26]J. H. Weaver, M. Grioni, J. J. Joyce, and M. del Guidice, Phys. Rev. B 31, 5290 (1985); M. Grinoi, J. J. Joyce, and J. H. Weaver, ibid. 32, 962 (1985).

[27]P. E. Schmid, Helvetica Phys. Acta 58, 371 (1985); W. Monch, Phys. Rev. Lett. 58, 1260 (1987).

[28]T. Kendelewicz (unpublished).

[29]L. J. Brillson, R. E. Viturro, M. L. Slade, P. Chiaradia, D. Kilday, M. K. Kelly, and G. Margaritondo, Appl. Phys. Lett. 50, 1379 (1987).

[30]J. L. Freeouf and J. M. Woodall, Appl. Phys. Lett. 39, 727 (1981).

[31]D. Troost, L. Koenders, L.-Y. Fan, and W. Monch, J. Vac. Sci. Technol. B 5, 1119 (1987).