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**Fundamental Studies of the Morphology, Chemistry, and Electrical  
Properties of Metals on GaAs and other III-V Semiconductor Compounds**

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The Study under the DARPA/ONR contract N00014-89-J-1083 resulted in 76 papers published in refereed journals and addressed a large spectrum of issues. The main results of these studies will be summarized below. More details can be found in original publications.

#### A. III-V surface passivation

A large effort has been placed to understand and develop passivation for the III-V surfaces. Although the major objective of these studies, to develop practical passivation for III-V devices other than heterojunctions (e.g. AlGaAs), is still unresolved (due to chemical instability of coatings in atmosphere) large progress in the understanding of many basic phenomena has been made. Our studies concentrated on two avenues. Firstly we explored the use S based solutions ( $\text{Na}_2\text{S}$ ,  $(\text{NH}_4)_2\text{S}$ , etc.) which markedly reduce surface recombination at the GaAs(100) surface. Secondly we studied the Sb interlayers on both GaAs and InP surfaces as an intermediate reaction barriers for the passivating layer.

##### a. sulphur coatings

This easy to apply method has been discovered few years ago at Bell labs and has attracted a large attention of the surface science community. The major issue is the mechanism of surface recombination velocity reduction. Unfortunately the practical objective of reducing time degradation of the performance has not yet been met. We have shown that, contrary to the prior believes, the S coatings do not reduce but increase the band bending on the n-GaAs(100) surface. The apparent contradiction of this phenomenon with the strong reduction of the surface recombination velocity (as measured by increased photoluminescence) achieved for this treatments, was successfully explained by us using the defect model of Spicer which pre-dates the development of S passivation. In this model,  $\text{As}_{\text{Ga}}$  and  $\text{Ga}_{\text{As}}$  antisite defects govern the electrical properties of the interface. It was concluded that although S treatment does not substantially reduce the total density of the surface states, it nevertheless drastically reduces surface recombination because of the change of in the surface stoichiometry (decrease of the  $\text{As}_{\text{Ga}}/\text{Ga}_{\text{As}}$  density ratio and  $\text{As}_{\text{Ga}}$  density) and the reduction of the efficiency of  $\text{As}_{\text{Ga}}$  recombination caused by the increased band bending. This mechanism is drastically different from what occurs at the Si/SiO<sub>2</sub> interfaces where the number of recombination centers is always kept low. Additionally, we

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have examined in detail the chemical reaction taking place for sulphur treated interfaces (particularly for simpler  $(\text{NH}_4)_2\text{S}$  treatment) and pointed out the importance of the Ga-S interface bond in explaining electrical properties of these interfaces (decrease of As concentration at the interface is required to explain photoluminescence) and in particular in resolving the issue of time stability. The existence of this bond was overlooked in prior studies which wrongly postulated an idealized GaAs/As<sub>2</sub>S<sub>3</sub> like interface. Our photoemission result clearly shows that As<sub>2</sub>S<sub>3</sub> is very unstable against annealing and leaves the surface as a unit. This explains an apparent As deficiency for this surface passivation. Attention has been also placed to understand reactions of S coated surfaces with metallic overlayers.

#### **b. Sb interlayers**

We also applied monolayer of Sb to passivate GaAs(110) and InP(110) surfaces. This work was initiated by the observation that a monolayer of Sb saturates all surface dangling bond states. Since the unsatisfied Ga dangling bond states are believed to be the source of the clean surface reactivity the Sb termination (in form of the zig-zag chains) chemically "passivates" the surface and limits chemical reactions (We stress that this microscopic meaning of the word passivate is perhaps different than in device application, where chemical passivation is linked resistance to atmosphere, a macroscopic phenomenon). Also, at least for InP, the Sb covered surface appears to unpin which can be linked to the reduction of the mid-gap states and implies electrical passivation. For GaAs the status is less obvious. However, since we were to move the surface Fermi level towards the flat band condition on both n- and p-type GaAs by annealing we conclude that the Sb/GaAs interface appears to be at most only lightly pinned. Additionally, we found evidence that monolayer of Sb reduces uptake of oxygen by an order of magnitude. This indicates that chemical reactions are indeed slowed down on the Sb covered surfaces. The hope was that chemical reactivity can be also reduced on metal covered surfaces with Sb interlayers. For GaAs this expectation was only partly confirmed by the data. While for less reactive metals (Al, In, Au) the interaction was impeded by interlayers, no such effect has been seen for strongly reactive metals like Pd. In the latter cases, reaction driven by the heat of the compound formation fully destroys the interlayer. Contrary to what we find for InP (see below) the Fermi level positions for metals on GaAs with and without interlayers are similar. The real test of passivation by Sb interlayers will come from applying an insulating layer to Sb terminated surface. One of the characteristics of device passivation is its ability to prevent carriers from entering the interface which is achieved by applying wide band-gap

material. We believe that a two stage termination in which Sb defines the interface electrically and the insulator provides wide gap termination can be of great value. This research is now in progress as unfounded work initiated by this proposal. The use of Sb and Bi interlayers has been particularly successful for InP interfaces. For InP, Sb interlayers give possibility to control reactions and Schottky barrier heights. Monolayers of Bi or Sb have been shown to act as buffer layers against oxidation reducing uptake by orders of magnitude. Core-level studies indicate that the Sb or Bi interlayer must be itself oxidized before there is strong oxidation of the InP. Some other results will be outlined below.

## **B. Ohmic contacts to GaAs**

Most GaAs interfaces are mid-gap pinned. However in recent years there has been increasing number of papers reporting changes of the Fermi level position accompanying changes in interface parameters of importance to device and their application. In our work we focused on the possibility of changing Fermi level position at GaAs interfaces and its implications in devices.

Using core level photoemission spectroscopy, we studied in detail the formation of the model GaAs/Pd-Ge contacts which are grown epitaxially and yield good interface morphology and long term stability. The aim of our experimental study was the determination of the band bending in correlation with interface chemistry and morphology. To achieve this goal, specific products of interface reaction were studied in simplified systems. This included model studies of the Pd/Ge, Pd/GaAs and Ge/GaAs interfaces. Interfaces were formed by the deposition of layers of Pd and Ge on the n-GaAs substrate and subsequent anneal. The deposition sequence was varied to allow a more quantitative determination of the role of each element. For low coverage we did not find a dramatic reduction of the barrier height. The barrier is found to be between 0.62 and 0.95 depending on the growth sequence and other details. The low resistivity of this contacts has been explained in the literature in terms of the thin heavily doped layer in the GaAs surface. We made theoretical and computer simulations showing that the heavy doped layer model is incompatible with the experimental temperature dependence of the contact resistivity and that some extrinsic transport mechanism should be considered to account for the experimental results.

A reduction of the barrier height to 0.62 eV was obtained when Pd is deposited before Ge and after anneal at 350 °C. Prior to the anneal, a 0.97 eV barrier, typical for the Pd/GaAs interfaces, is obtained. The corresponding interface chemistry suggests that this 0.35 eV lowering can be described by a model in which interface states are compensated by charge from As n-type dopants in the Ge layer. Both Waldrop and Grant and Bauer et al. have seen similar barrier height movement for Ge deposited directly on GaAs (100) in the presence of excess As, but this is the first evidence that this effect takes place in an actual ohmic metallization. The result for Pd deposited first contrasts sharply with the stable barrier height observed for the case where the Ge was deposited first. In this second system, a constant barrier of 0.75 eV was found after every process. While in both cases, a Ge-GaAs heterojunction exists at the interface, there is a much smaller amount of As in the overlayer when Ge is deposited first, due to the much more limited interaction between the overlayer and the substrate. As a result, there was much less As available to dope the Ge first contact layer heavily n-type.

Some attention have been placed to study In contacts to GaAs which also often display Ohmic behavior after annealing in formic gas or atmosphere. Contrary to prior suggestions we found no indication of InGaAs graded heterojunction formation. In fact we find that under vacuum conditions the barrier height is close to 1 eV independent of annealing. The annealing causes only a slight increase of ideality factor in the I-V measurement. We conclude that formed under vacuum condition In/GaAs contacts are not Ohmic.

### **C. High Schottky barriers on n-InP**

While the formation of Ohmic contacts and stability of Schottky barriers are main concerns for n-GaAs, the problems in devices using n-InP involve the inability to form high Schottky barriers which typically have values of 0.5 eV or less. We have shown that this problem can be solved by the use of Sb interlayers. For example, an unusually high barrier of 0.82 eV has been observed for the Au/n-InP interface with Sb interlayer. The same contact without interlayer yielded barrier of only 0.5 eV, a common value for many n-InP interfaces. The Sb covered surface prior to the metal deposition gives nearly flat band condition for both n- and p- type of doping with residual band bending as low as 0.2 eV. The photoemission data indicate that, for the gold overlayers, Sb interlayer completely inhibits surface chemical reactions. Similar results have been found for Pd, Cu, Al and Ag. Although Schottky barriers for this metals are in a 0.3 to 0.55 eV range, they increase to

between 0.49 to 0.82 eV when Sb interlayers are used. Similar results have also been obtained with Bi interlayers.

Core level photoemission spectroscopy has been used to investigate interfacial chemistry at Ag and Au/InP(110) interfaces with one monolayer thick Sb interlayers. Although changes in the line-shapes of the In 4d and P 2p core levels do not indicate presence of substantial chemical reactions within the substrate, the comparison of the attenuation profiles of these core levels suggests that P atoms are more apt to segregate into the overlayer than In atoms. This noticeable asymmetry in outdiffusion affects the Schottky barrier heights of interfaces. As for the interlayer, large changes of the line-shape of the Sb 4d indicates reaction its with metallization. The presence of reaction is confirmed by a more detailed analysis. The data suggest that, although the epitaxial morphology of Sb monolayers on InP(110) stongly affected by deposition of Au and Ag, the presence of the Sb interlayer strongly prevents strong chemical reactions between the substrate and metallization which is particularly strong for the Au/InP interface without interlayers. Specifically for InP interfaces first passivated with one monolayer of Sb, the Au-In alloying is completely inhibited.

The important issue of thermal stability of Au and Ag/n-InP interfaces with increased Schottky barriers (0.8 eV) has been also studied with photoemission. Strong clustering is observed as a result of annealing of both interfaces. This alone suggests a reduction in the reaction between overlayers and substrates in comparison with interfaces without Sb interlayers. Change in the Fermi level positions due to annealing is measured for both interfaces to be less then 0.1 eV for up to 300° C. However, segregation of In atoms into the Ag overlayer is observed above 300° C at Ag/Sb/InP interfaces, and a small pinned component with a level at 0.4 eV below CBM appears above 200° C at the Au/Sb/InP interfaces. In summary: Schottky barriers are found to be stable up to at least 200° C. Optimization of the passivation condition might further improve the thermal stability of these Schottky barriers.

The annealed Ag interfaces on Sb covered p-InP give an anomalously low Schottky barrier of 0.5 eV.

#### **D. Electronic structure and Schottky barrier formation on GaAs (100) prepared by thermal desorption of a protective arsenic coating**

##### **6**

Soft x-ray photoemission spectroscopy has been used to characterize MBE grown GaAs (100) surfaces and interfaces which have been prepared by the thermal desorption of a

protective As coating. The samples studied were grown and arsenic capped identically to those used in a previous study of Brillson. In this previous work, "unpinned" Schottky barrier formation was reported, with barrier heights over a wide (0.75 eV) range. This is a striking result, as it was previously believed that all metals will pin GaAs surfaces in a narrow energy range near midgap. This large range of barrier heights later led to the suggestion that the (100) surface could become an insulating layer which could screen out the effects of MIGS. Motivated by this work, we studied Al and Au Schottky barriers since the deposition of these two metals gave the extreme low and high barriers in the 0.75 eV range. We have also characterized the clean surfaces prepared by desorbing the As caps at different temperatures. The As 3d and Ga 3d core levels showed that the surface stoichiometry could be varied significantly with the desorption temperature. The As 3d lineshape was found to be the best indication of the surface stoichiometry after the anneal. The valence band spectra did not show any strong features due to the excess As which could be used to determine when the sample was completely decapped. The electronic structure of the surface layer was investigated experimentally, and no evidence of an insulating reconstruction was found. In our study of band bending, we found that the low doped samples which were used here and in Brillson study showed significant photovoltages resulting in incorrect band bending measurements. We also found that the Au measurements are made difficult by the presence of core level shifts due to Au-Ga alloying. After solving the problems with the photovoltages and alloying, we found that the barriers heights for Au and Al differ by only 0.25 eV.

#### **E. Metallization and promotion of oxidation and nitridation by alkali overlayers**

A large effort has been devoted to study reactions of the alkali metal on surfaces of semiconductors. The alkali metal (AM) overlayers display many unique adsorption properties. The prior research resulted in a wealth of practical applications most of which utilize the fact that submonolayer quantities of AM cause a large reduction of the substrate work function. In fact, under certain condition, when deposition of AM is followed by dosing with oxygen, the work function can be lowered to the extent that the vacuum level at the surface falls below the conduction band in the semiconductor. This so called negative electron affinity interfaces have applications in high efficiency emitters, infrared detectors, image intensifiers and spin-polarized electron guns. Despite wide range of applications, not all processes at the AM covered surfaces are understood. We conducted a large scale investigation of these interfaces with particular emphasis on the mechanisms of the

Schottky barrier formation and AM-enhanced oxidation and nitridation (which could be of interest in microelectronics).

We find that despite extremely low work function, submonolayers of the AM yield Schottky barriers in the value range of other metals. In view of the fact that metals work functions (WF) vary by several eV, this observation is by large contrary to what might be expected from the Schottky model sometimes invoked in the literature to explain barrier height vs metal WF behavior. However, we note that, within the class of AM, there is small but distinctive dependence of the band bending on the WF. Specifically on n-doped GaAs the band bending for Cs is found to be the largest, for Na the smallest, with values for K and Rb in between. A reversed trend is found for the p-doped substrates. While AM chemisorption at room temperature is often limited to one atomic layer, multilayers can be absorbed at reduced temperatures. This allows to follow the development of the overlayer metallicity for overlayers with controllable growth and morphology. The development of the overlayer metallicity has been followed by monitoring the evolution of the Fermi level cut-off and free electron plasma losses. It is found that it becomes metallic for coverages well in excess of one monolayer at which coverage the pinning positions for n- and p-doped GaAs substrates coincide which can be explained by metallic screening of defects and metal induced gap states. In the context of the mechanism of the Schottky barrier formation, the role of the donor states introduced by AM overlayers was strongly emphasized.

Core level photoemission experiments have been performed to study the effect of AM overlayers on oxidation and nitridation of Si, Ge and III-V semiconductors. At room temperature, the presence of an alkali monolayer enhances oxidation by orders of magnitude. This behavior is reverse to what we see for Sb interlayers. On Si a rapid thermal annealing at moderate temperatures results in formation of the Si-SiO<sub>2</sub> interface. The catalytic mechanism is found to be nonlocal in nature. A similar behavior is found for nitridation using molecular nitrogen which results in formation of Si<sub>3</sub>N<sub>4</sub> at the Si surface after moderate anneal which also removes the AM catalyst. Also for InP and GaAs, the presence of AM interlayers affect reaction with oxygen and nitrogen. While clean surfaces of this semiconductors remain unaffected by molecular N, the AM interlayers induce large nitrogen uptakes and cause formation of complex nitrides. These are the first examples of promoted nitridation for semiconductors.

#### **F. Various aspects of Schottky barrier formation.**

The basic issue in Schottky barrier studies is the understanding of the mechanisms responsible for the phenomenon. From the point of view of applications, the most important issues are barrier height control and contacts time stability. It is clear that all these problems are interconnected. The defect model developed by Spicer over the last decade relates changes of the barrier heights in GaAs Schottky contacts to changes in the interface stoichiometry; specifically to the As/Ga density ratio. The supposition that stoichiometry controls the Fermi level movement by affecting abundances of defect states has been tested by us with success for a range of practical systems. Specifically we concluded that on n-GaAs the barrier increases for As deficient (or Ga rich) interfaces and that the reverse is true for p-doped GaAs. Conversely As rich interfaces display lower barriers on n-GaAs. In the process of these investigations it became obvious that some other mechanisms, in particular metal induced gap states, have to be considered in particular at the low temperature formed or nonreactive interfaces. In fact, the dual nature of the pinning was stressed by us in several papers.

A widely discussed paper by Hecht [M. H. Hecht, J. Vac. Sci. Technol. B 8, 1018 (1990)] have drawn attention to low temperature (LT) Schottky barrier formation studies of metal / III-V interfaces. This paper have pointed out that when photoemission spectroscopy (PES) is used to determine band bending, the light used in the measurement can influence this band bending through the photovoltaic band flattening. The effect is particularly strong at LT. Consequently many of the conclusions drawn from earlier LT studies have now been questioned. A careful reevaluation of our data indicate that most of our studies is not affected by this effect. For example, we reevaluated the band bending overshoot phenomenon, a behavior observed on high-doped p-GaAs which shed important light on the low temperature chemisorption and found interesting model and theoretical explanations. On the basis of photoemission data we conclude that, contrary to Hecht's suggestion, the overshoot is intrinsic to the low coverage barrier formation process. Hecht's hypothesis that the overshoot is due to photon-induced charging of the GaAs surface fails to explain the following key aspects of the data. (1) The overshoot is dependent on the temperature of the interface formation and its influence on adatom clustering rather than the temperature at which the measurement is made. (2) The degree of overshoot has a simple dependence on the adatom ionization potential and electronegativity. (3) The overshoot is observed on very high doped substrates in which tunneling is anticipated to restore any nonequilibrium surface charge. We suggest that the model involving adsorbate-induced donor states at the overshoot level in the gap provides a more

straightforward and complete explanation of these and other aspects of the overshoot data. Hecht's work is instrumental in pointing out the role of light in the reduced band bending observed for the LT low-doped interfaces. However, it appears that the overshoot is a real effect, related to the position of surface states in the semiconductor gap and is not an artifact related to the measurement process.

A Poisson integration program has been used to study the potentials around small (comparable in size with to the semiconductor depletion length) metal clusters on semiconductors. The lateral extent of the band bending from the cluster edges has previously been estimated using a simple one-dimensional depletion length  $x_{1d}$ , but our more detailed analysis determines that lateral depletion length, is intrinsically shorter than the depletion depth into the bulk. Furthermore, the depletion edge shrinks in all direction as the cluster size fall below  $x_{1d}$  for any given substrate doping. For a 100 Å diameter cluster on  $5 \times 10^{17} \text{ cm}^{-3}$  n-doped GaAs, the lateral potential change is 90 % complete at a distance of 190 Å from the cluster edge, whereas  $x_{1d}$  is 460 Å. The intercluster potential variation was calculated for known cluster morphologies in order to quantify the effect of the lateral potential variation on substrate core level lineshapes and energy positions. When the clusters are separated by more than lateral depletion length, broad areas of minimum band bending constitute most of the uncovered surface, while the regions of full band bending are isolated to the cluster edges. However, the overall potential barrier development as measured by photoemission is significantly faster. Thus sources of intercluster charge states such as submonolayer coverages of either adatoms or substrate defects have to be considered. For example, isolated chemisorbed adatoms have been proposed in the past to induce band bending on p-GaAs, and such adatoms should be detected between clusters in the imaging methods employed to date (SEM and RHEED).

Our studies of InP interfaces have ascertain basic differences between this substrate and the more intensively studied GaAs substrate. For overlayers as different as Sn, Ge, O, Sb, and Mg, we observed a reversal of the band bending on the n-doped substrates from 0.4 eV at one half monolayer coverage to near flatband conditions for thicker overlayers. Such effect is not seen on GaAs (with exception of Sb). Consistently with this Ohmic behavior on n-InP, we have measured (I-V) large barrier heights (almost 1.3 eV, nearly a band gap) for thick overlayers of these materials on p-InP. These results, particularly the difference between the InP and GaAs band bending, cannot be explained in the context of the MIGS model. We proposed an extension of the defect model to InP with defects energies consistent with the theoretical calculations and other experimental data. This model, which

uses an additional donor level just below the CBM, is also consistent with our observation that annealing of the clean p-InP pins the Fermi level close to CBM. Annealing is known to preferentially sublimate P which leads to the formation of vacancies.

We also studied with photoemission ten selected overlayers on GaP(110). We find that despite differences in reactivity, the Fermi level is stabilized near 0.8 eV above VBM with little dependence on the type of the overlayer. Hence the barrier heights exhibit a much weaker relationship to the overlayer work function than reported previously by Brillson. As with GaAs and InP, the GaP Fermi level position is in the range of defect levels as created by irradiation and theoretical charge neutrality level toward which MIGS should move the Fermi level.

We have also performed a first study which uses resonant photoemission to better understand reactions at the transition metal semiconductor interfaces. The data were taken close to the Ni 3d to Ni 3d threshold at Ni/GaAs interfaces and compared with results from NiAs crystals. The data clearly indicate a presence of profound chemical reactions taking place for thin overlayers at room temperatures and for arbitrarily thick overlayers after annealing.

#### **G. Photoemission studies from ordered (epitaxial) interfaces.**

Semiconductor core level lineshapes and binding energy shifts as determined by computer fitting programs provide detailed information on the bonding configuration and morphology of both the clean surfaces and interfaces. Because every atom in a distinct environment has a specific core level energy, the information on bonding geometry now available from structural tools can be complemented by photoemission. Initially we have used ordered overlayers to suppress semiconductor surface components and thus obtain quantitative information on the intrinsic lineshape parameters of the substrate core level spectra. Our results demonstrate that in many cases the intrinsic line width is much narrower than previously believed. One example of this is our work on the Si(111)2x1 surface. The complex reconstruction of this surface has been hypothesized by Pandey in his  $\pi$ -boded chain model. Using epitaxial Ge overlayers to attenuate the surface shifted components, we were able to obtain the lineshape parameters of a single Si 2p component. Fitting the clean surface Si 2p with components of this lineshape then accounted for all the surface atoms in the Pandey model. Analysis of the component intensities proved that the

data agree well with the predictions of the model. Similar studies to establish surface core level shifts were conducted for the Ge(111) surface and for surfaces of III-V semiconductors.

We have used Sb and Bi overlayers to obtain the lineshape parameters and surface shifts for InP, GaP, and GaAs. Detailed determination of the III-V interface band bending requires consistent fitting for many overlayers and coverages with such reliable parameters. We have also found on these ordered interfaces that, while the substrate core level spectra offer information on the average potential over the surface, the overlayer core level spectra provide a local probe of the surface Fermi level position at the isolated atoms, small islands, and/or two dimensional patches that form in the early stage of interface formation.

All ordered systems studied with high resolution photoemission spectroscopy have also been studied with SEXAFS. The atomic geometries determined by SEXAFS were correlated with results of the photoemission studies. For example, a monolayer of Sb removes the surface components from semiconductors and this corresponds to the saturation of the dangling bonds in the adsorption geometries displayed by these atoms in the structural models proposed.

#### **H. Structural characterization of interfaces: Surface extended X-ray Absorption Fine Structure of adsorption geometry.**

SEXAFS experiments have been performed for ordered overlayers of Sb and Sn on various semiconductor surfaces. Specifically, Sb monolayers have been prepared on Si(111)7x7, Si(111)2x1, Si(100)2x1, Ge(111)2x1, GaAs(110)1x1 and GaP(110)1x1, while Sn monolayers have been studied on Si(111)2x1 and Ge(111)2x1. The data for Si and Ge provide information relevant to epitaxy on these substrates, and furthermore these data facilitate the analysis of the more complex interfaces on the III-V semiconductors. For example Ge has similar backscattering characteristics to Ga and As. Similarly Si studies assist in the analysis of the phosphorous-containing III-V's. In the process of these experiments we have developed a new sample-current method for detecting total yield signal and constructed a new fluorescence detector based on the Si/Au pin diodes which was successfully tested and applied. The analysis of the Sb on Si(111) and Ge(111) data indicates that Sb forms trimers or zigzag chains with the substrate-Sb and Sb-Sb distances close to the sum of the covalent radii. Formation of chains is also observed on the (110)

surfaces of III-V semiconductors. Our analysis indicates that Sb on (100) surfaces of Si forms dimers which reside in alternating fourfold hollow sites between the substrate dimers. Again, distances are close to sums of the respective covalent radii. The bonding geometry from SEXAFS has been confirmed by our STM results. The STM, with lateral resolution on the order of 2 to 3 Å, provides direct real space views of the surface geometry that in most cases can be easily interpreted. Although STM can provide the long range order of the surface with little difficulty, it lacks the ability to measure bond lengths easily measured by SEXAFS, and it cannot determine adatom-substrate coordination except in certain cases. Because of this a combination of STM and SEXAFS is particularly useful for studies of the adsorption geometries at interfaces.

Our experience with SEXFAS has led to the development and application of Soft X-ray Standing Wave Technique to studies of the interface geometry. We applied soft X-ray standing-wave technique (XSW) to study geometrical structure of ordered monolayers of Sb overlayers Si(111) and GaAs(110). Using the back-reflection diffraction geometry from (111) or (220) planes, we determine the perpendicular distances of Sb atoms to the substrate and compare these with theoretical calculations and ELEED determinations. The various models of Sb chemisorption are evaluated on the basis of our data. The XSW technique is an ideal complement to the STM studies because it can easily establish perpendicular distances. XSW can also provide the complete adatom geometry if a set of independent diffracting planes is used. Additional advantages of the XSW exist. For example: 1. The mathematical analysis of the data is relatively simple. 2. There is little constraint on the overlayers which can be studied. 3. The photon energy is scanned in only a narrow range around a Bragg peak. This line research is continued with great success in our current studies.

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