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# Structure, electronics and dynamics of clean and metal adsorbed semiconductor surfaces: recent results and perspectives

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## Abstract

Here, we present a few examples, largely reflecting our own contribution, which reveal novel interesting phenomena uncovered at well characterized semiconductor surfaces, essentially thanks to detailed synchrotron radiation studies. Clean surfaces as well as surfaces covered with sub-monolayer films of unreactive metal adsorbates are selected to highlight peculiar *structural features*, such as surface and/or sub-surface dimerization at InAs(100) surfaces, subtle *electronic states*, i.e. adsorbate-induced quantized two-dimensional electron gas at InAs surfaces and ultra-fast *dynamical behaviours*, such as the flip-flop motion of buckled dimers on the (100) face of group IV semiconductors.

(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

High energy and momentum resolution are crucial for photoelectron spectroscopy (PES) studies of surfaces in the vacuum ultraviolet (VUV) and soft x-ray region, while a high flux in the hard x-ray region is mandatory for surface x-ray diffraction (SXR) investigations. This is currently obtained at third generation synchrotron radiation (SR) facilities where typically the high brilliance of the source also permits us to achieve spatially resolved spectroscopic imaging with photoelectrons [1]. The time resolution necessary to study dynamical processes on a femtosecond scale, already pioneered at such facilities [2], will presently be reached in the near future at fourth generation, fully coherent, sources, such as the x-ray free electron laser in development at DESY, Hamburg, Germany (TESLA project) [3].

Our knowledge of semiconductor surfaces and interfaces [4] has largely relied on the advanced characterization tools and methods developed at SR facilities. The electronic and

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atomic structures of the most important group IV and III–V semiconductor surfaces and the early stages of their interface formation with several metals are nowadays well understood thanks to the synergetic use of SR techniques and real space local scanning probe microscopies (SPM) in combination with advanced theoretical methods. To illustrate some of the recent achievements in this wide field, we will select a few examples, which reflect to a large degree our own contribution to this progress.

Until quite recently the determination of the atomic arrangements of the surface reconstructions of the (001) surfaces of the III–V compound semiconductors has been a real challenge. Detailed knowledge of the atomic geometry of these surfaces is particularly important since a wide variety of high-speed electronic and optoelectronic devices used in communications technology are fabricated on (001) wafers. A unique model involving sub-surface dimerization of the group III atoms for the metal rich  $c(8 \times 2)$  superstructures has just been found by SXRD using direct methods [5], slightly before we could resolve, also by SXRD, the atomic structure of the As-terminated  $\beta 2(2 \times 4)$  surface where we have instead found As dimers in the top layer [6]. These atomic structures will be described in section 2.

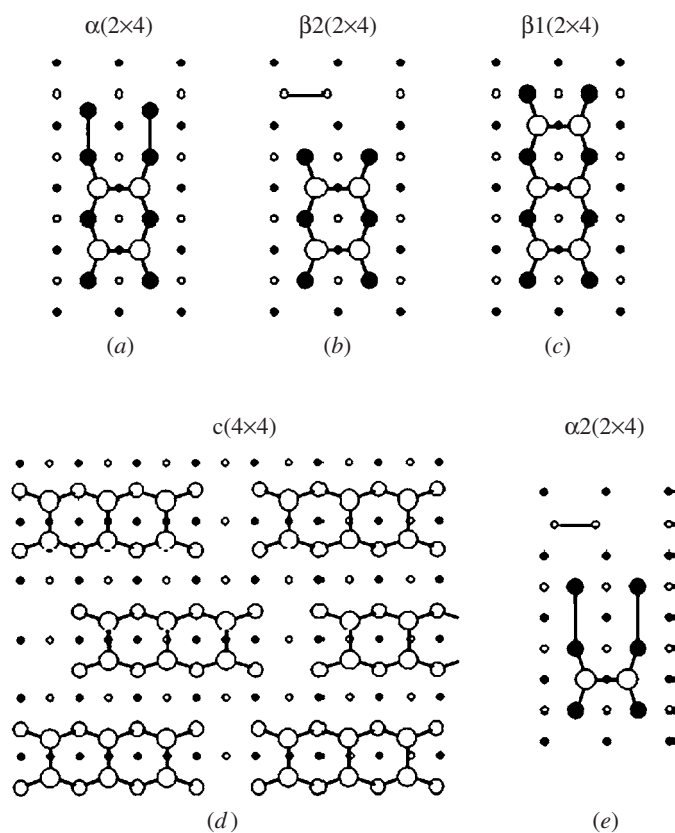
In the last few years, the metal-induced two-dimensional electron gas (2DEG) located in the near surface region at InAs surfaces has attracted much attention. This is both for fundamental reasons [7, 8] and in view of technological applications: hybrid structures that incorporate 2DEGs are involved in Josephson transistors (i.e. Nb on InAs substrates [9]) as well as spin transistors (ferromagnetic materials on InAs substrates [10]).

Synchrotron radiation angle-resolved photoelectron spectroscopy (ARUPS) has been the key experimental technique to obtain detailed and direct information on the formation of the 2DEG. In section 3 of this paper we will recall that we achieved the highest Fermi level jump above the InAs conduction band minimum (CBM) in a controlled way by depositing cesium adsorbate atoms onto the cleaved (110) surface [11]. This led to the formation of a 2DEG located close to the surface [12]. Furthermore, we could directly measure the dispersion of the quantum states within the created electron channel [13].

Silicon surfaces have been extensively studied both experimentally and theoretically due to their major technical importance for semiconductor devices. It is well established that at the very (100) surface pairs of atoms form buckled dimers. The  $p(2 \times 1)$  structure observed at room temperature (RT) is due to the flip-flop motion of these asymmetric dimers. Their dynamics at low temperatures is presently studied experimentally by scanning tunnelling microscopy (STM) [14, 15]. At high temperatures new molecular dynamics simulations have been carried out, extrapolating to a dimer flipping frequency of  $\sim 3 \times 10^6$  Hz at RT [16]. The corresponding timescales can be compared to many physical, chemical and biological processes that are by nature dynamic and take place on the timescale of molecular vibrations, typically around 100 fs. X-ray experiments to study structural changes that occur on such a time scale are an emerging area of research in condensed matter physics at third generation SR facilities [2]. X-ray free electron lasers (FELs) will give a fantastic impetus to such investigations. Hence in the framework of the Technical Design Report of the TESLA project at DESY (Hamburg, Germany) we have proposed as a fundamental study the structural observation of the dynamics of the dimers on the silicon(100) surface [17, 18]. This proposal will be summarized in section 4.

## 2. Atomic structures of the As-rich and In-rich InAs(001) surfaces

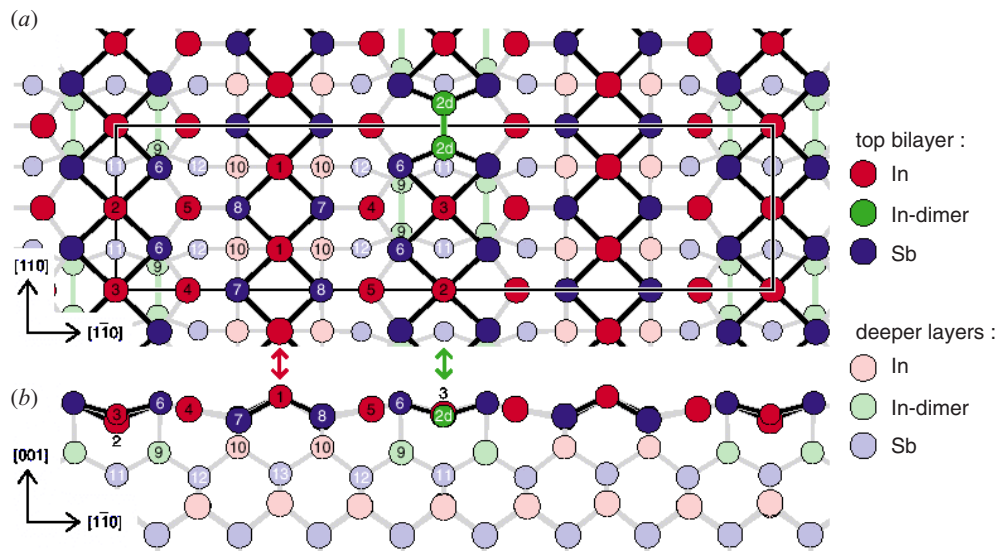
The (001) surfaces of III–V compounds show a wealth of reconstructions that have challenged the scientific community until very recently. Knowledge of their atomic structures is extremely important since these surface reconstructions play a crucial role in both homoepitaxial and heteroepitaxial growth, e.g. during the fabrication of a large variety of high-speed electronic and optoelectronic devices used in communication technologies.



**Figure 1.** Structural models proposed for the group V rich (100) surfaces. The open circles represent group V atoms, and the filled circles group III atoms.

We could determine the full three-dimensional (3D) atomic geometry of the molecular beam epitaxy (MBE) prepared As-rich InAs(001)  $2 \times 4$  reconstruction by SR-SXRD [6]. The analysis of a large set of non-equivalent in-plane diffraction peaks and several out-of-plane rods yields, among different models previously suggested, the so-called  $\beta_2 - (2 \times 4)$  structure proposed by Chadi [19], shown in figure 1. This structure comprises two As dimers in the top layer and one trench As dimer in the third layer below the first incomplete In layer, as for the corresponding GaAs(001) superstructure [20]. The stability of this  $\beta_2 - (2 \times 4)$  structure for InAs(001) has been further confirmed by STM and density-functional theory calculations [21].

Using STM we have previously investigated the  $(4 \times 2)/c(8 \times 2)$  reconstruction of the In-terminated InAs(001) surface prepared by ion bombardment and annealing (IBA). This surface appeared as very smooth and well ordered with wide terraces ( $\geq 500 \text{ \AA}$ ) across which uninked lines extended over large distances [22]. We attributed these lines to first layer dimer rows in agreement with the  $\beta_3$ -model suggested by Ohkouchi and Ikoma [23] which contained one top-layer and two second-bilayer dimers. However, a very recent determination of the atomic structure of the  $c(8 \times 2)$  reconstructions of InAs-, InSb- and GaAs-(001) surfaces by SR-SXRD using direct methods converges toward a new unique geometry common to the III-rich (001) surface reconstructions of the III-V semiconductors [5, 24]. The model, which is in agreement with recent density functional theory (DFT) calculations, low-energy electron



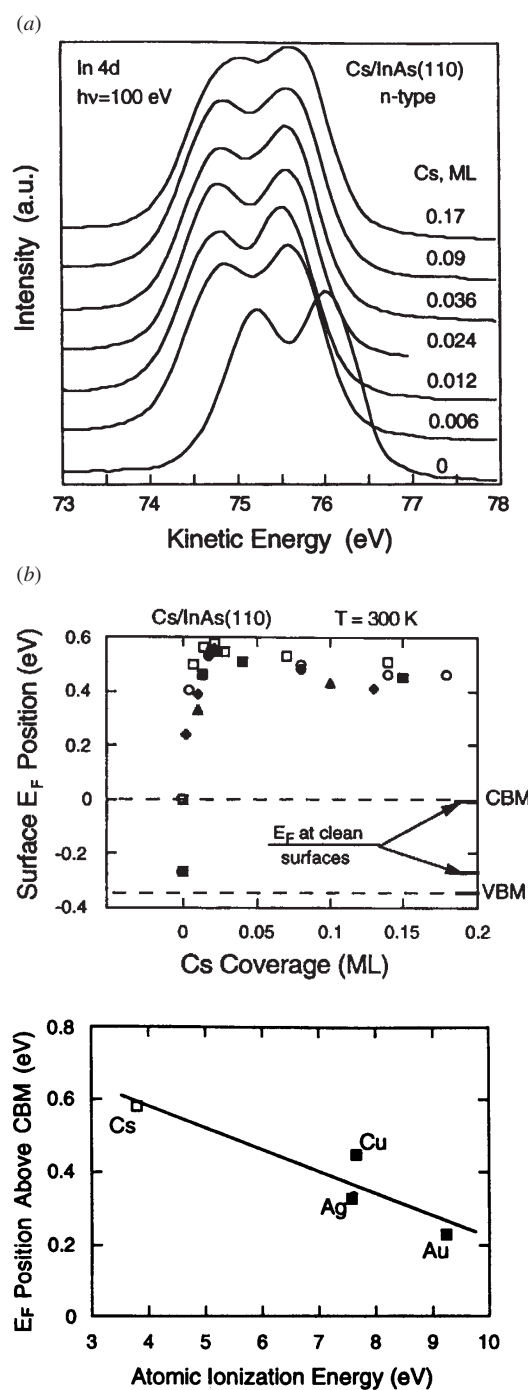
**Figure 2.** Structural model (adapted from figure 2 of Kumpf *et al* [5]) derived for InSb(001)- $c(8 \times 2)$  viewed from (a) the top and (b) the side. Indium dimers are coloured green. The labels correspond to important atoms in the structure (see [5]).

diffraction (LEED) measurements and simulated STM images in the case of GaAs [25], is displayed in figure 2. It consists of sub-surface dimers of group III elements in the second bilayer and linear chains of atoms located at non-bulk sites at the surface along the  $[110]_{\text{bulk}}$  direction with a decreasing tendency to dimer formation within the chains with increasing atomic weight of the compound.

To conclude this section we emphasize that if for group V rich (001) surfaces group V dimers have been clearly identified to be the basic building blocks of the  $(2 \times 4)/c(2 \times 8)$  reconstructions, contrary to common belief, the main constitutive moieties of the  $(4 \times 2)/c(8 \times 2)$  reconstructions of the group III rich surfaces are not dimers on the surface but sub-surface dimers in the second bilayer. Finally we also stress that the direct methods which enable full *ab initio* surface structure determination in three dimensions [26], and thence eliminate the need to guess starting models for the structural refinement, constitute a novel invaluable tool in SR surface x-ray crystallography.

### 3. Cs-induced quantized 2DEG at the InAs(110) surface

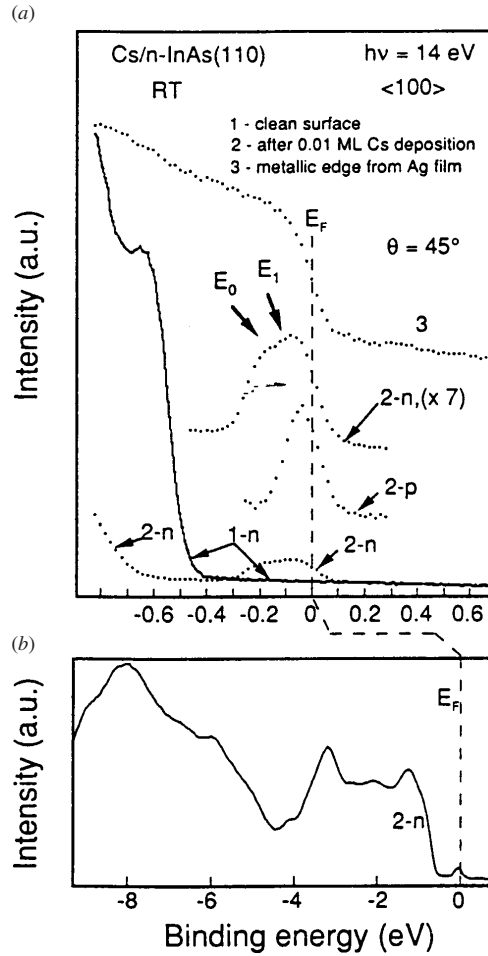
Recently, by measuring with SR-PES the band bending changes upon adsorption of small amounts of Cs at RT on *in situ* cleaved InAs(110) surfaces, exhibiting originally flat band conditions, upon following the shifts of the In 4d and As 3d core levels (see figure 3(a)), we have found that we can adjust the position of the Fermi level  $E_F$  at the surface from the top of the valence band/bottom of the conduction band (VBM/CBM), for p/n-type samples, up to 0.6 eV above the CBM, for about 0.01 monolayer (ML), for both types of bulk doping [11]. Furthermore, upon deposition of various metals, we have also noticed an inverse proportionality between the maximum  $E_F$  shift induced by the adsorbate and its ionization energy (see figure 4). The pinning of  $E_F$  at a high position above the CBM leads to a strong downward band bending, thus creating inversion or accumulation layers according to the doping type, that is a 2D electron channel situated just beneath the surface.



**Figure 3.** (a) Normalized In 4d core level spectra of the Cs/n-InAs(110) interface at increasing Cs coverages; the energy shifts of these spin-orbit split core levels with respect to the spectrum of the bare surface reflect directly the band bending changes resulting from the metal adsorption. (b) Fermi level positions at the InAs(110) n-type (open symbols) and p-type (closed symbols) surfaces as a function of Cs coverages at RT. These positions with respect to the band edges are derived from such measurements as shown in (a); different symbols correspond to different samples.

**Figure 4.** Measured highest positions of the Fermi level on InAs(110) with respect to the CBM for different metal adsorbates as a function of their first ionization energies.

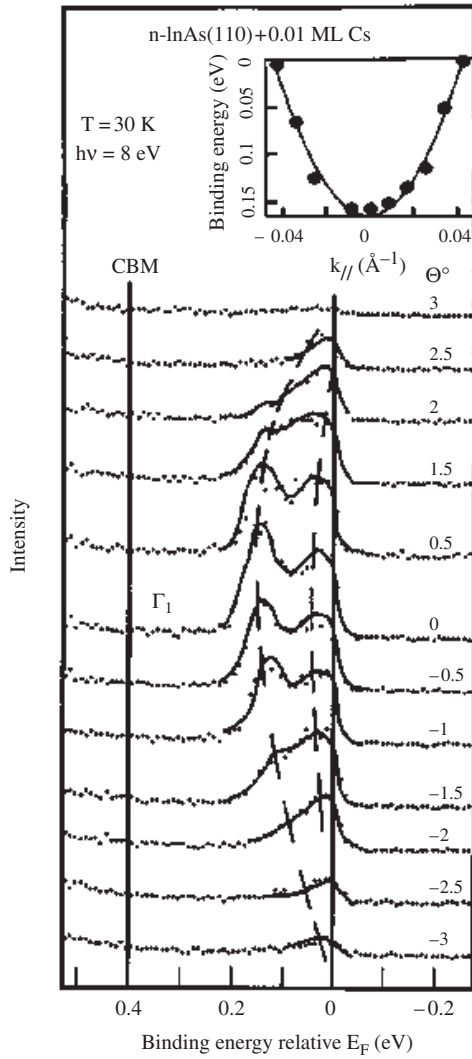
In a first study, performed at RT in an essentially *angle-integrated mode* at a photon energy of 14 eV, we detected a small photoemission feature appearing near  $E_F$  inside the normally empty conduction band, in the close vicinity of the  $\bar{\Gamma}$  points of the first and second Brillouin zone with an intensity of about one order of magnitude less than that arising from the valence



**Figure 5.** Angle-integrated spectra in the vicinity of  $E_F$ , measured at the  $\bar{\Gamma}$  point of the second Brillouin zone of: (a) (1 - n) the bare InAs(110) surface; (2 - n) after deposition of  $\approx 0.01$  ML Cs at RT; (2 - p) same as 2 - n, but taken for a  $p$ -type sample; (3) Fermi edge from an Ag film, (b) full valence band spectrum (2 - n) after deposition of  $\approx 0.1$  ML Cs at RT.

band (see figure 5). We ascribed this feature to emission from the 2D channel and interpreted it in the framework of the surface doping model considering the charge neutrality condition, i.e. identifying the dopant with a donor-level  $E_D$  of a single adsorbate atom located at the maximum of the energy position of  $E_F$  above the CBM [27]. Using self-consistent solutions of the Schrödinger and Poisson equations we derived the potential well shape, the electron energy levels and the charge distribution below the surface. In this way we could demonstrate that this feature arose from two occupied discrete energy levels within the channel, resulting from quantization along the surface normal [12].

Later we performed a subsequent study [13], at low temperature (LT) (30 K) in order to reduce the phonon broadening contribution in the spectra, in an *angle-resolved mode* with a  $0.5^\circ$  resolution to reach a high momentum ( $k_{\parallel}$ ) resolution and at a lower photon energy of 8 eV to further increase the probed depth due to the very low kinetic energies of the outgoing photoelectrons, since we calculated that the maximum density within the 2D channel was located at about 50 Å below the top surface for the deepest energy level  $E_0$ . In these conditions, in a narrow phase space around the  $\bar{\Gamma}_1$  point, we could resolve the individual quantized states and measure their dispersions as a function of  $k_{\parallel}$ . In such a way we determined the average effective mass,  $m^* = 0.05m_0$  ( $m_0$  is the free electron mass), of the carriers for motion parallel



**Figure 6.** PES spectra taken from the 2DEG at different emission angles along the  $\Gamma-\bar{X}$  direction in the vicinity of the  $\Gamma_1$  point of the InAs(110) surface. The dispersion of the deepest electronic state,  $E_0$ , as a function of  $k_{||}$  is shown in the inset.

to the surface in what clearly turned out to be a high mobility 2DEG within the sub-surface channel (see figure 6).

Electron accumulation or inversion layers have not only been detected by SR-PES at InAs(110) surfaces; they were also observed by ARUPS at clean InAs(100) and (111) surfaces prepared by IBA or by MBE growth (homoepitaxy) [28] as well as by heteroepitaxy on GaAs(111) substrates [29]. In this last case, Friedel oscillations of the 2DEG, in the 2D sub-band state quantized in the surface accumulation layer, were directly observed in real space at LT around point defects or inside a stacking fault tetrahedron by  $dI/dV$  mapping performed simultaneously with topography in the conduction band [30].

We note that we also found a 2DEG by ARUPS on the InAs(100) surface upon lead adsorption [31], on the InAs(111)B surface upon Cs, Pb and Sn adsorption [32] as well as on another narrow bandgap semiconductor surface: *in situ* cleaved InSb(110) samples upon Cs adsorption at RT [33].



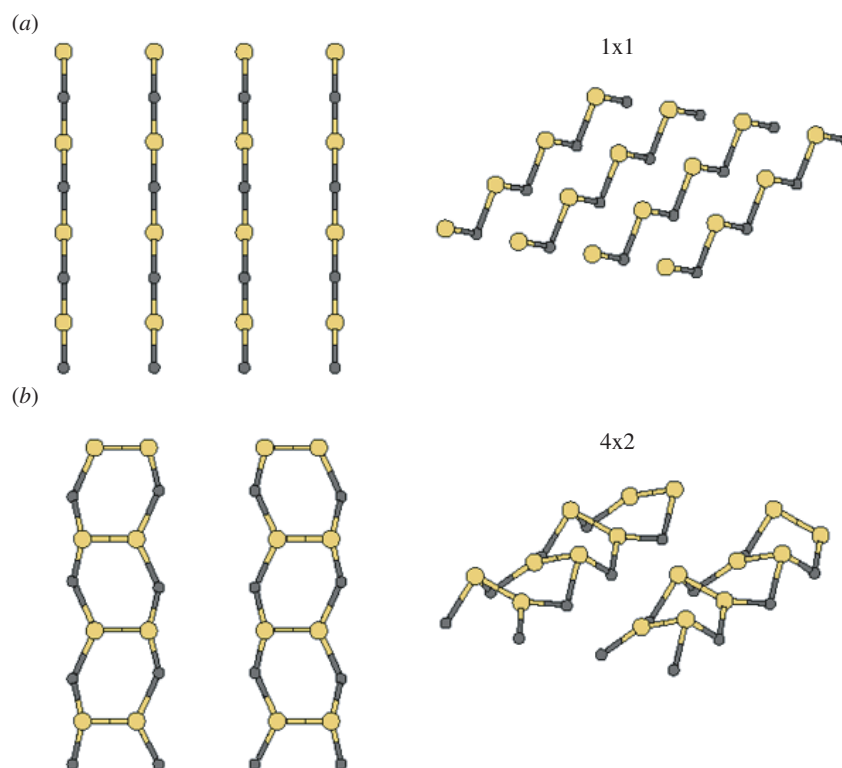
#### 4. Dimer dynamics on the silicon(100) surface

Si(100) is considered as one of the most important solid surfaces, from both scientific and technological points of view; it has a particular role in surface physics, especially due to its microelectronics applications. Many different aspects of this surface have been the subjects of numerous theoretical and experimental works, especially by SR [34]. It is well established that pairs of top Si atoms form dimers along the  $[01\bar{1}]$  direction. These dimers are the building blocks of the different superstructures; their origin and nature is one of the most intensively discussed issues in surface physics. The surface dimer rows are maintained up to 1463 K, while the measured melting temperature is 1680 K [35]. These dimers are tilted and the  $p(2 \times 1)$  structure observed at RT is due to the thermal activated flip-flop motion of these asymmetric dimers. At low temperatures, below about 200 K, the  $p(2 \times 1)$  structure is reversibly transformed into the  $c(4 \times 2)$  structure. The structural transformation is described as an order-disorder phase transition: the  $c(4 \times 2)$  structure results from the freezing of the buckled dimers with alternated configurations of the tilt angles, as in a simple 2D antiferromagnetic ordering, depicted in figure 7. Until the beginning of 2000, this  $c(4 \times 2)$  reconstruction was considered as the ground-state structure, although practically degenerate with the  $p(2 \times 2)$  configuration, which consists of an out-of-phase and an in-phase ordering of the buckled dimers along and perpendicular to the dimer rows [36]. In STM images taken at about 100 K, the  $c(4 \times 2)$  reconstructed surface appears as a zigzag pattern of dimers rows. This wiggling along the rows reflects the alternate orientations of the buckled dimers; it disappears above the phase transition temperature. Typically at RT the dimers look symmetric because only their time average position can be observed upon STM imaging.

It was thus quite a surprise to recover, upon further cooling the  $c(4 \times 2)$  surface below about 20 K, a new  $p(2 \times 1)$  arrangement of, apparently, symmetric, unbuckled dimers in two independent STM observations at temperatures down to 5 K [37, 38]. Indeed this recent discovery could eventually question the current common belief about the stability of the asymmetric dimers at the zero temperature limit. Besides, the two groups gave conflicting interpretations of this surprising observation. This was either in terms of a sort of re-entrant flipping motion of the *asymmetric* dimers giving a dynamically active surface phase as at RT [37] or, on the contrary, as the evidence of the stabilization of static *symmetric* dimers [38]. In fact symmetric dimers have not been completely excluded by theorists, they could possibly be stabilized either by an antiferromagnetic coupling between dimer spins [39] or by an electronic correlation between the dimers [40].

Hence we see that this new discovery raises challenging questions, although tip effects in STM imaging may play a major role [14].

Experimentally a key issue is the direct observation of the flip-flop motion of the buckled dimers in the course of a dynamical study of this Si(100) $2 \times 1$  surface. This motion could be inferred *only indirectly* (i) in the course of a SR-SXRD structural study at RT, since it is hardly distinguishable from a static disorder among the buckled dimers [41], or (ii) upon comparison of the deconvolutions of the Si 2p spectra in high resolution SR core level spectroscopy at RT for the  $2 \times 1$  phase and at LT for the static  $c(4 \times 2)$  phase yielding very similar line shapes and decompositions [42]. We note in passing that the same situation is met in the case of Ge(100) which presents the same type of reconstruction and a similar phase transition at about 220 K. A comparison on the one hand of SXRD data acquired at RT [43] and at 150 K [44] and on the other hand of SR photoelectron spectra (valence bands and Ge 3d core levels) from both phases [45] again yields only an indirect indication of the dynamical motion of the dimers. The situation is even worse for the diamond-like phase of tin ( $\alpha$ -Sn). There the presence of asymmetric dimers on the (100) surface displaying a  $2 \times 1$  LEED pattern at RT has just been

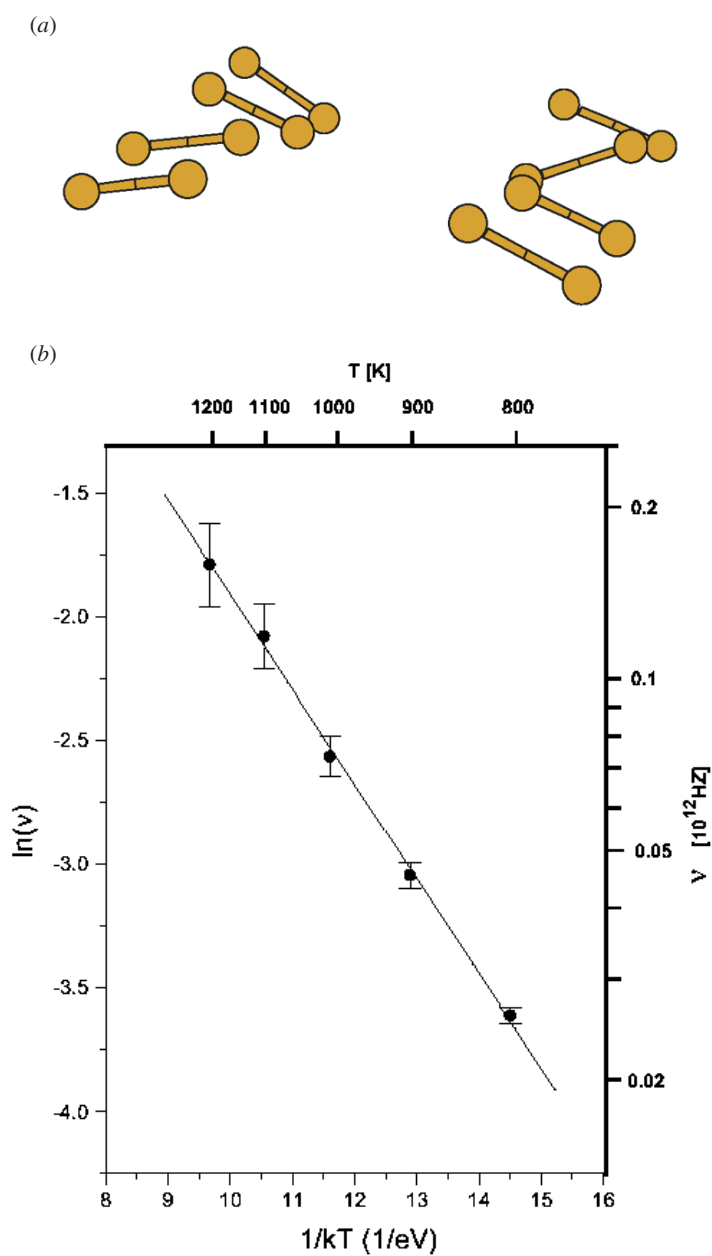


**Figure 7.** Ball and stick bilayer model of (a) the unreconstructed Si(100) $1 \times 1$  surface, and (b) the  $c(4 \times 2)$  structure. The left panels show top views, and the right panels show side views. The large circles represent topmost surface atoms and the small circles second-layer atoms.

demonstrated recently by SR-PES of the valence bands and of the Sn 4d core level [46], but no LT data are presently available.

Hence the direct observation of the dynamical flip-flop motion of the buckled dimers at the (100) surfaces of the group IV semiconductors is presently too demanding. Yet it will be possible, as revealed by new molecular dynamics simulations at high temperatures [16–18], with the fourth generation x-ray FELs. These simulations give at each temperature the time evolution of the geometry of the dimers from which one can extract their frequencies of flipping; an example is given in figure 8(a) which displays an instant snapshot of the configuration of eight dimers after a 40 ps run at 1000 K, starting at  $t = 0$  from an initial  $c(4 \times 2)$  arrangement as in figure 7(b). These demonstrate that typically with the extremely high brilliance and the time structure of the 1 Å x-ray FEL at DESY (trains of bunches, each of 90 fs giving bursts of  $10^{12}$  photons, separated by 93 ns intervals) a complete structural dynamics study of the Si(100) surface will be possible in a very large temperature domain spanning from typically 5 K—where the puzzling issue of the symmetric or asymmetric geometry of the dimers will be addressed and solved—up to at least 1400 K.

To conclude this section we admit that the planned study may look somewhat academic. Yet we should keep in mind that several other semiconductor systems also present intriguing dynamical behaviours. This is indeed the case for the analogous clean Ge(100) surface, probably also for the  $\alpha$ -Sn(100) surface, but also typically for important metal/semiconductor couples. Presently one of the hottest topics in semiconductor surface science concerns the



**Figure 8.** (a) Instant snapshot of the configuration of the buckled dimers after a 40 ps simulation run at 1000 K (see [16]). One can observe three reversed positions and notice different length and tilt angles of the dimers. (b) Arrhenius plot,  $\ln v$  as a function of  $1/kT$ , for temperatures between 800 and 1200 K, obtained from the flipping frequencies of the silicon dimers on the  $\text{Si}(100)2 \times 1$  surface.

dynamics of the  $\sqrt{3} \times \sqrt{3}$  reconstructions induced by one third of a ML of tin or lead adsorbed on silicon and germanium (111) surfaces and the nature of the reversible LT phase transition to the ground-state  $3 \times 3$  structure [47,48]. Success in carrying out such experiments and solving

such fundamental issues will open up the way to many other experiments of practical interest. One could envisage, for example, studying the diffusion of the dimers at high temperatures for better control of silicon growth by MBE.

## 5. Summary

We have presented a few significant examples of the major role of SR investigations in the determination of the structural and electronic properties of clean, e.g. InAs(001) and Si(100), and metal adsorbed, e.g. Cs/InAs(110), semiconductor surfaces of paramount importance from both fundamental and practical points of view. We have underlined the crucial impact of high-resolution photoemission of the valence bands in angle-resolved ultraviolet PES and put strong emphasis on core level spectroscopy in the soft x-ray region. These advanced spectroscopic tools have permitted the determination of novel and subtle phenomena such as the creation of a quantized 2DEG in the close vicinity of the (110) surface of indium arsenide upon adsorption at RT of small amounts of cesium. In the hard x-ray region, we have stressed the importance of grazing incidence x-ray diffraction. It is undoubtedly an extremely powerful tool to obtain reliable atomic geometries of semiconductor surface reconstructions that have challenged the scientific community until very recently, such as the structures of the (001) surfaces of the III–V compounds.

Finally, we have drawn novel perspectives for the study of dynamical processes on a femtosecond timescale. In this respect let us mention that *time*- and angle-resolved pump-and-probe PES measurements based on an amplified short-pulse (150 fs) titanium:sapphire laser system have been used to study the electron dynamics and accumulation at the cleaved InAs(110) surface [49, 50]. High temporal resolution in the femtosecond regime can presently be reached only with such pulsed laser sources. The development of fourth generation sources, such as Linac-based FELs, will permit us to add the femtosecond time resolution to the high spatial resolution already available in this energy range at third generation SR facilities. Typically a new source, the TESLA test facility in Hamburg, will soon deliver coherent synchrotron light, up to 200 eV, with 150 and even possibly 30 fs pulse lengths [3]. It will be opened to users, firstly, soon (within two years) in the soft x-ray region, and secondly, in the following years, in the hard x-ray region down to one angstrom or even less. Such sources will open completely new avenues: dream experiments will become feasible in practice by combining in a synergetic way very high *time*, *energy*, *momentum* and *spatial* resolutions.

## Acknowledgments

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