The study of surface adsorbed C_{60} molecules with metastable impact electron spectroscopy and UPS (He I) ☆

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Abstract

Metastable impact electron spectroscopy (MIES) in combination with UPS (He I) is applied to study the electronic properties of surface adsorbed C_{60} molecules. The growth of C_{60} layers on clean, thermally oxidized and cesiated Si(100) is monitored by recording the spectra of the electrons ejected during the layer growth at room temperature. The various mechanisms for electron ejection during the interaction of photons and He* metastables with C_{60} are discussed. The results furnish also information on the interaction between the studied Si(100)-based substrates and the C_{60} adsorbates.

Keywords: Amorphous thin films; Auger ejection; Electron emission; Fullerenes; Photoemission

1. Introduction

Metastable impact electron spectroscopy (MIES), in particular in combination with UPS (He I), has proved its capabilities to:
- study the local electronic structure of individual surface atoms on the outside of surface layers,
- observe changes in the electronic structure during the growth of surface layers [1], and
- detect changes in the molecular orientation of surface adsorbed molecules [2].

In this work we apply the combination of MIES and UPS to study the electronic properties of C_{60} molecules adsorbed on clean, thermally oxidized (20 Å) and cesiated (one complete adlayer) Si(100) surfaces. Until now only one study with MIES of C_{60} multilayers (on Cu(100)) has been published [3]. The electron spectroscopic techniques are employed here in order to study the layer growth during the exposure of various silicon-based surfaces to fullerenes starting from the freshly prepared surface up to a coverage of several C_{60} layers. The motivation for this work is the study of

(1) The possible mechanisms for electron ejection in the interaction of the metastable atoms with surface adsorbed C_{60} molecules, namely (i) Auger processes, such as Auger capture (AC) and Auger deexcitation (AD) (surface Penning ionization) involving two (AC) or one (AD) electron from the C_{60}, respectively, and (ii) collective modes for C_{60} excitation,

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☆ Dedicated to the occasion of the 65th birthday of Professor Ch. Schlier.
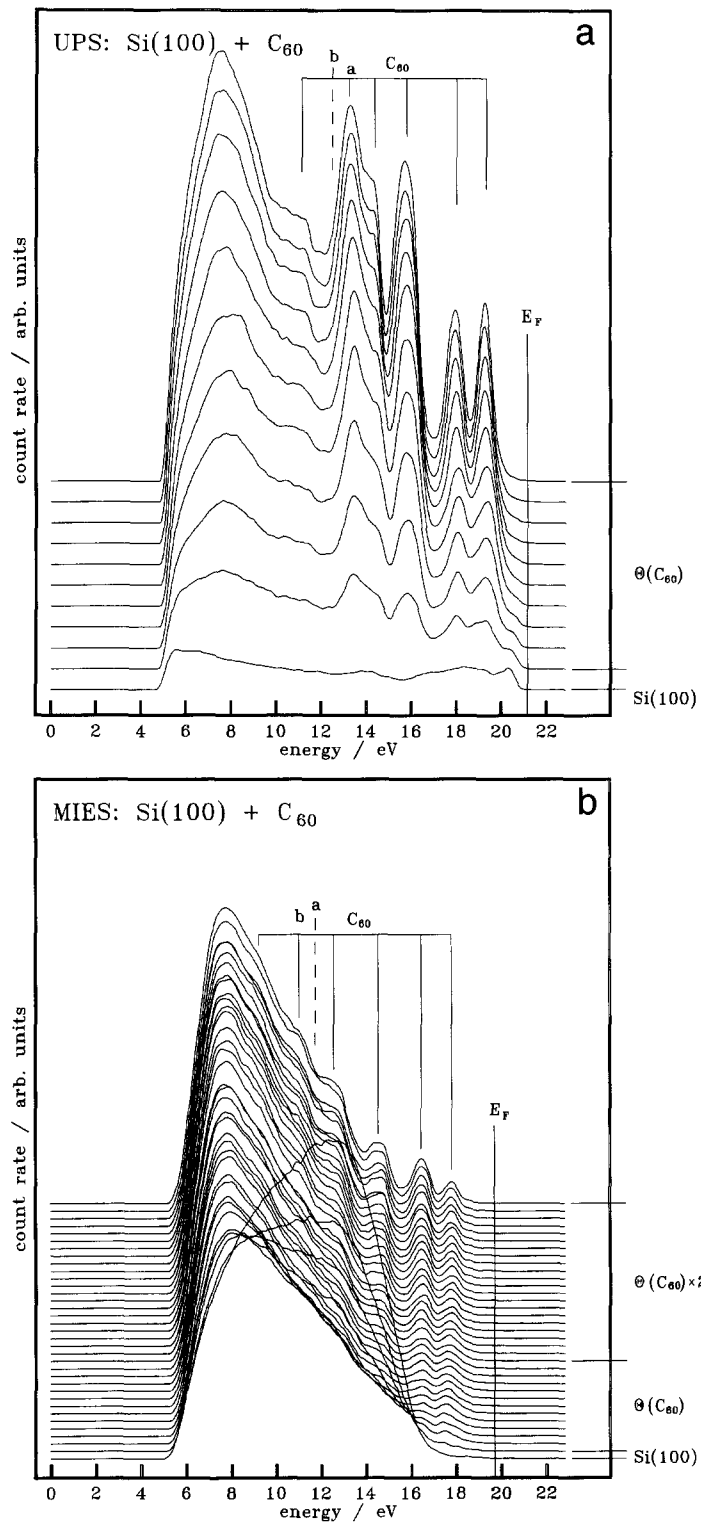* Corresponding author.

Fig. 1. UPS (a) and MIES (b) spectra recorded during the exposure Θ of Si(100) to C_{60} at room temperature; bottom curve is for uncovered Si(100).
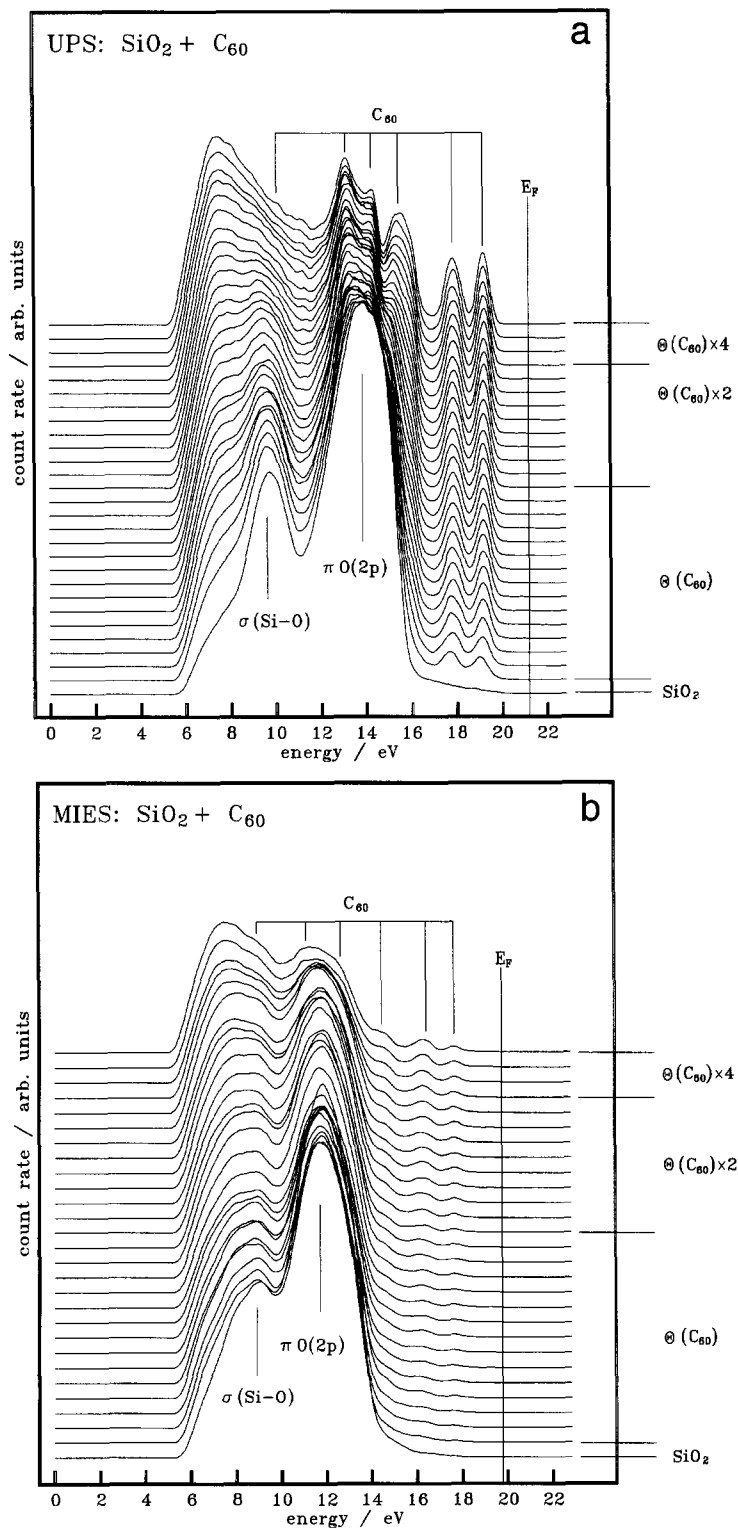
Fig. 2. As in Fig. 1, but for the exposure Θ of thermally oxidized Si(100) to C_{60}.

as the excitation of a giant plasmon resonance followed by its decay by electron ejection [4–6].

(2) The interaction between conducting or insulating substrates and single C_{60} molecules adsorbed at these surfaces.

Our study is a prerequisite for the investigation of chemical reactions involving C_{60} at surfaces. The combined application of MIES and UPS appears to be well suited to distinguish between the formation of exo- and endohedral complexes [7]. In addition, the combination of these techniques has the potential to give information on the growth of passivating C_{60} layers on various substrates, such as a protective barrier against water contamination [8].

2. Apparatus

The apparatus was described previously [1]. Briefly, a cold cathode He gas discharge serves both as source for an intense He metastable beam (for MIES) and as He I photon source (for UPS). He metastables and He I photons are separated by means of a time-of-flight technique. The incidence angle of metastables and photons is 45 deg with respect to the surface. The electron energy spectra are recorded under 90 deg with respect to the surface. The time required to collect a complete spectrum is 1 min for both MIES and UPS. Both spectra are recorded quasi-simultaneously by utilizing suitable counting techniques. Electrons emitted from the Fermi level appear at 21.2 eV in the UP spectra; because of the 1.4 eV smaller excitation energy of the He metastables (19.8 eV for He(2 ^{3}S)) this emission appears at 19.8 eV in the MIE spectra. The energy at which electrons originating from the Fermi level appear in the photoemission or Auger deexcitation spectra (in MIES) is denoted by E_F. The low energy cutoffs in the MIES and UPS spectra give directly the change of the work function of the surface as function of the exposure to C_{60}. In the following binding energies E_b refer to the Fermi level E_F.

The Si(100)-based substrates were prepared in the following manner: an n-doped (Sb; 0.02 $\Omega \cdot$ cm) Si(100) surface was cleaned by several cycles of annealing to 1300 K. An oxide layer of 20 Å thickness was produced by heating the clean Si(100) surface for 3 h at 1000 K in an oxygen atmosphere

of 10^{-7} mbar (exposure 10^4 L). Cs atoms from a SAES Getters Inc. dispenser source were offered to the Si(100) surface at room temperature. The layer growth was monitored by MIES/UPS; details can be found in Ref. [9] (see also Fig. 3).

C_{60} molecules were evaporated from a Knudsen cell (filled with C_{60} powder, Hoechst AG, "High Grade S", 99.4% C_{60}) operating at 603 K in the UHV chamber. During the operation of the cell with C_{60} or of the Cs dispenser source the pressure in the UHV chamber remains below 3×10^{-10} mbar during Cs and 2×10^{-9} mbar during C_{60} exposure. All measurements were performed at room temperature.

The spectra shown in the Figs. 1–4 were collected in the following manner: at constant exposure rate Θ (the same in all figures) spectra were recorded in equal time intervals. When the spectra started to show only minor changes upon further exposure, the time interval between consecutive spectra was increased (doubled for 2 Θ etc.). At present we are not able to make an accurate calibration of the thickness of the adsorbed layers. However, for C_{60} deposited on Si(100) it is known [8] that only one adlayer remains on the substrate after heating to 900 K. From a comparison of Figs. 1 and 4 we can roughly estimate that the 4th spectrum from the bottom represents one complete adlayer on Si(100).

In Figs. 3 and 4 Cs atoms were offered to the surface at constant exposure rate. In Fig. 3 the exposure was stopped when the work function of the surface started to saturate. Thus, the bottom spectrum of Fig. 3 represents the saturation coverage by Cs obtainable at room temperature.

3. Experimental results

3.1. C_{60}/Si(100)

About 50% of the C_{60} induced photoemission (Fig. 1a) in the topmost spectrum appears to be caused by single electron ionization. This contribution has been identified previously as ionization of the highest occupied π- and σ-type MOs. The positions and relative intensities of the photoionization features agree well with those reported in Ref. [10] for UPS (He I) for C_{60} films (for a summary on photoemission studies on fullerenes see Ref. [11]).
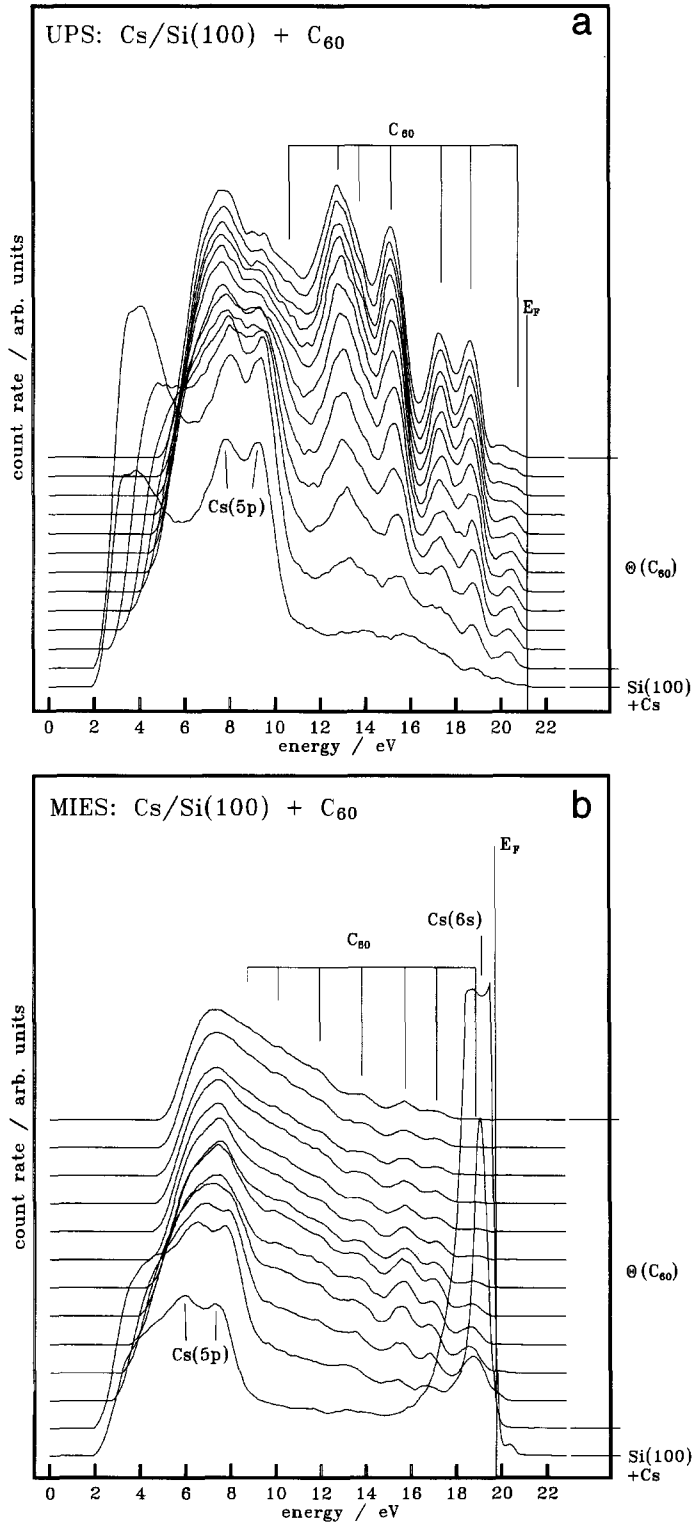
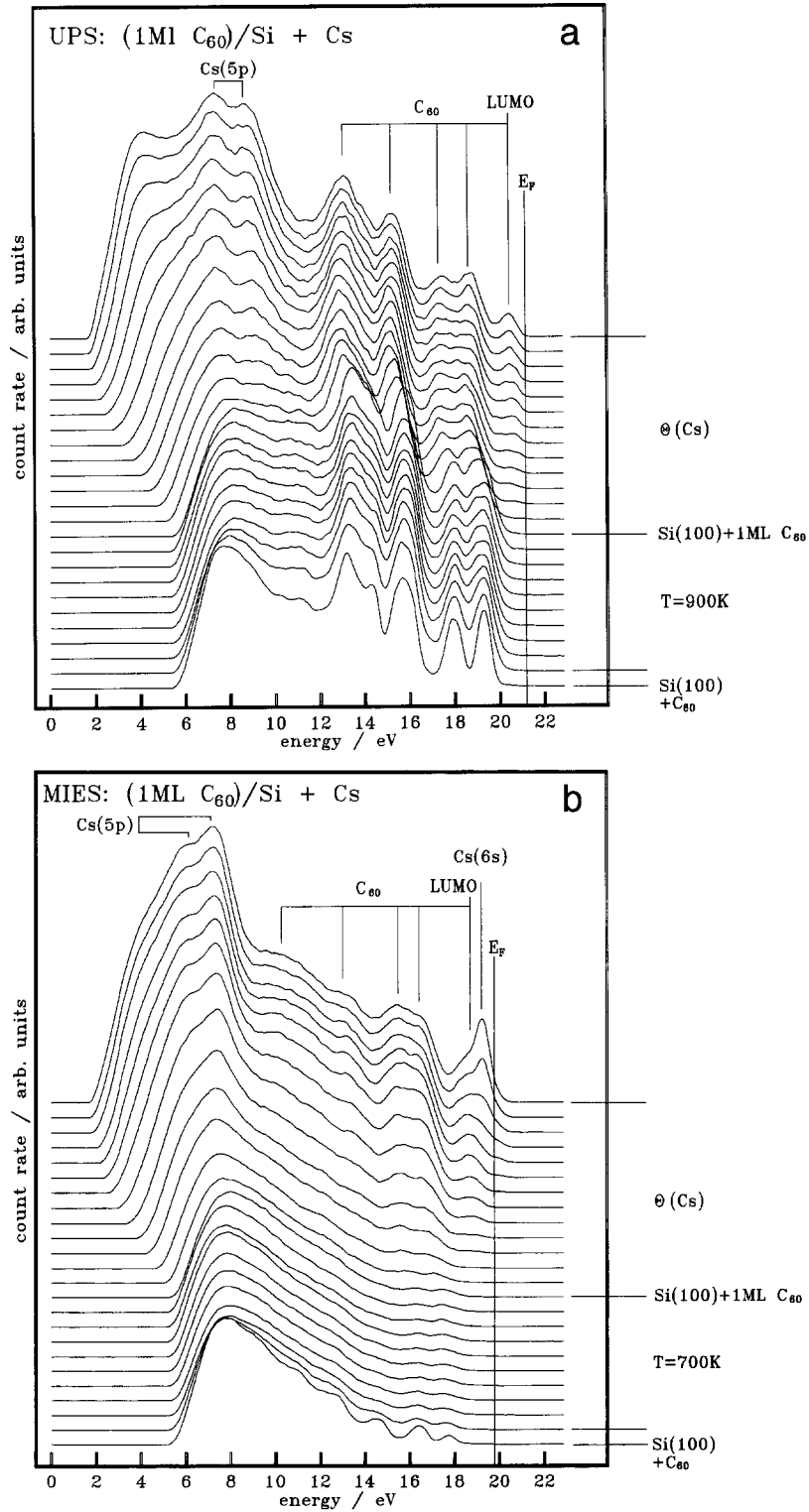Fig. 3. As in Fig. 1, but for the exposure Θ of cesiated Si(100) to C_{60}.

Fig. 4. As in Fig. 1, but obtained during the heating of a C_{60} film on Si(100) (spectra 1 to 11) followed by the exposure of the remaining adlayer to Cs.

EELS [5] and, in particular, photoionization data [4,6] show that for photon energies between 10 and 30 eV the *ion* signal primarily results from autoionization following excitation of a giant plasmon resonance of about 20 eV (for free C_{60} molecules). Unfortunately, at present no data appear to be available for the electron emission eventually originating from the autoionization process. At least part of the broad continuum contribution peaking at very low energies could be due to collective excitation followed by electron ejection. In this connection it is remarkable that the valence band spectra for photon energies larger than 40 eV [12] seem not to show the strong continuum contribution that we see with He I photons. Unfortunately, at present we cannot estimate the fraction of true secondary electrons in our spectra.

The bottom MIES spectrum in Fig. 1b is due to Auger capture of He^+ ions formed by the resonant transfer of the He 2s electron into the substrate. This process involves two electrons from the surface, and consequently the Auger capture spectrum is the self-convolution of the Si(100) surface density of states (SDOS) [13].

Similar discrete features as in the UPS spectra appear during the exposure to C_{60}. They are shifted towards lower kinetic energies by about 1.4 eV corresponding to the difference between the excitation energy of the He(2 ^{3}S) (19.8 eV) and the He I energy ($h\nu = 21.2$ eV). Therefore, these features are due to Auger deexcitation (surface Penning ionization) of He(2 ^{3}S) involving the highest lying occupied C_{60} MOs.

The features seen with MIES relate in general, but not always, to those seen with UPS: in particular, the strong feature, labeled **a** in Fig. 1, is seen only weakly with MIES. Instead, a shoulder, labeled **b** in Fig. 1, appears in MIES which is not clearly seen with UPS. These important differences will be discussed further in Section 4.

The discrete features discussed above account for less than 10% of the total electron emission; therefore it is unlikely that the broad continuum is due to true secondary electrons. In Section 4 we will show that the strong continuum emission underlying the discrete features can be attributed to Auger capture (following resonance ionization of He*) involving two C_{60} electrons.

3.2. C_{60}/SiO_2

The peak at $E_b = 7.5$ eV in the UPS spectra of Fig. 2a, denoted by πO(2p), is due to the ionization of the oxygen π-orbital at the SiO_2 surface while the emission at larger binding energies, denoted by σ (Si–O), involves the σ-orbital of the (Si–O) bond [14]. At least the emission labeled σ(Si–O) disappears practically entirely at the later stages of the exposure. The same C_{60} induced structures as in Fig. 1a appear in the UPS spectra, namely the single electron features and the underlying continuum. In the topmost spectrum the energetic position and relative intensities of the discrete features are similar as for $C_{60}/Si(100)$. However, some emission from the substrate appears to be present between 12 and 16 eV. During the growth of the layer the features at $E_b = 5.3$, 5.8 eV (e.g. from ionizing t_{2u}, g_u, h_u, h_g) appear at a relatively late stage of the exposure (as compared to those at $E_b = 2.3$, 3.7 eV).

As long as the substrate is still accessible to interaction with He*, the MIES emission (Fig. 2b) is strongly influenced by Auger deexcitation of He* involving the valence band of SiO_2. This produces emission similar to the features σ(Si–O) and π O(2p) seen with UPS although the emission from σ (Si–O) is now less pronounced [14]. In order for the Auger capture process to take place, the He 2s electron must be transferred to the surface. This process is inhibited because the He 2s level is in resonance with the bandgap of the substrate [14]. Upon C_{60} exposure the discrete features from the ionization of the C_{60} MOs develop gradually. The two π-derived peaks at $E_b = 2.3$, 3.7 eV are located in the bandgap of the substrate. Only the topmost MIES spectra start to resemble those obtained for $C_{60}/Si(100)$; however, the substrate induced emission never disappears completely.

3.3. $Cs/Si(100) + C_{60}$

During the exposure of Si(100) to Cs two peaks (labeled Cs(5p) in the bottom spectrum) develop in the UPS spectra of Fig. 3a which are due to the ionization of the Cs 5p fine structure states [13]. Details of the electronic structure of Cs/Si(100) utilizing MIES and UPS will appear elsewhere [9]. Upon C_{60} exposure of the cesiated surface the dis-

crete features (already discussed in Section 3.1 and
3.2) develop, although their binding energies are
larger by 0.8 eV. In addition t_{1u}, the former lowest
unoccupied molecular orbital (LUMO), becomes now
filled as signaled by the peak appearing about 1.6 eV
above the peak attributed to ionization of h_{1u} (see
also Refs. [15,11]). The emission from the ionization
of t_{1u} starts to disappear again upon further exposure
to C_{60}.

In the MIES spectra (Fig. 3b) the same two
features due to Cs 5p ionization appear upon expo-
sure to Cs. The strong emission near E_F labeled
Cs(6s) is due to the interaction of He*(2 ^{3}S) with
Cs 6s. It has been shown that Cs(6s) is mainly due to
autodetachment of the He^{-*}(1s2s^2) formed by the
resonant transfer of a Cs 6s electron to the projectile
[16–18]. Upon C_{60} exposure the Cs 6s emission
weakens, and simultaneously the features due to the
Auger deexcitation involving the C_{60} MOs appear.
They are now more pronounced than for C_{60}/Si and
SiO$_2$ indicating that more He*(2^3 S) atoms interact
with C_{60} via the Auger deexcitation process. As in
UPS emission from the occupied t_{1u}, the former
LUMO, is seen. The simultaneous disappearance of
the emission involving the Cs 6s valence electron
signals very directly the charge transfer from Cs to
C_{60} filling t_{1u}.

The topmost spectra display again the strong con-
tinuum contribution; the Auger deexcitation features
are now considerably weaker than during the initial
stage of the formation of the adlayer. The LUMO is
practically not occupied anymore in those C_{60} species
which the metastable can interact with.

3.4. C_{60} / Si(100) + Cs

In Fig. 4 a C_{60} adlayer deposited on Si(100) is
heated up to 800 K where only one adlayer remains
on the substrate (11th spectrum from the bottom) [8].
The C_{60} monolayer was then exposed to Cs atoms.
During the Cs exposure the surface work function
decreases to about 1.7 eV (see change in the low-en-
ergy cutoff of the spectra). The two fine structure
components from Cs 5p ionization appear in the
UPS spectra of Fig. 4a. Simultaneously with the
work function decrease the C_{60} induced features
shift by about 0.8 eV to larger binding energies, and

t_{1u} (the former LUMO) becomes gradually occupied
starting at a work function of about 4.2 eV.

The heating of the fullerite weakens the features
caused by Auger deexcitation in the MIES spectra of
Fig. 4b. Cs coadsorption causes emission from the
ionization of Cs 5p and C_{60} t_{1u}. During the cesiation
the features from Auger deexcitation become stronger
again. When the work function saturates, the Cs
adlayer displays metallic features: this is signaled by
the appearance of the feature (labeled Cs(6s)) due to
the presence of the Cs 6s electron at the location of
the Cs atom. Further exposure to Cs (not shown in
Fig. 4) leads to a strong increase of Cs(6s) similar to
what is seen for Cs/Si(100) (see Fig. 3b, bottom).

4. Discussion

4.1. Ioniziation mechanism

As pointed out in the previous section about 50%
of the photoionization (He I) results in continuum
emission rather than in discrete features as expected
for one-electron transitions. On the basis of the
energy dependence of the photoionisation yield as
reported in Ref. [4] for free C_{60} molecules, we
cannot exclude that part of the continuous contribu-
tion to the electron yield arises from autoionization
of a plasmon resonance centered in the region 20 to
27 eV photon energy, i.e. well above the C_{60} ioniza-
tion energy (7.54 eV). Unfortunately, we do not
know at present the yield for ejection of secondary
electrons under the studied conditions. A more de-
tailed discussion of the continuous part of the spectra
may demand for photoion–photoelectron coinci-
dence data; they could establish which fraction of the
electron emission is caused by autoionization.

Normally it is found that MIES spectra from
surfaces with large work functions (larger than about
4 eV) are dominated by electrons from the Auger
capture process. It was however suggested that the
strong continuous part seen in the MIES spectra
from C_{60} films could in part be due to electron
ejection following the formation of a plasmon reso-
nance [3]. In order to test this proposition we have
simulated the MIES top spectrum of Fig. 1b with the
method proposed in Refs. [19,20]; it was successfully
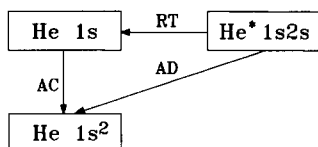applied to the simulation of electron spectra obtained

Fig. 5. Reaction scheme for He* collisions with C_{60} adlayers. RT: Resonant electron transfer. AD: Auger deexcitation (surface Penning ionization). AC: Auger capture (neutralization).

Fig. 6. Simulated and experimental MIES spectra for C_{60} on Si(100) (topmost spectrum in Fig. 1b).

in He* and slow He+ collisions with clean [20] and alkali covered [21] metals, and LiF films [22]. Briefly, a reaction scheme describing the sequence of processes during the interaction of the He* with the adlayer must be selected (see Fig. 5). A set of coupled rate equations, one for the occupation number of each involved state, must be solved during the projectile's path in the vicinity of the surface. Reasonable choices must be made for the rates describing the transitions between the involved states and their energies as a function of the projectile–surface distance. Distance dependent interaction potentials between the He projectile and the C_{60} adlayer as well as rates for the resonant and Auger processes are obtained in the following way (see Refs. [19,20] for details):

- it is assumed that the He levels become modified mainly by the image interaction when the projectile approaches the surface, and
- the transition matrix elements are approximated by the overlap of the wavefunctions of the surface and the projectile. Transitions can involve all those surface states which are energetically accessible to Auger processes.

The density of states (DOS) in C_{60} films was calculated using various approaches [23–25]. Fig. 6 shows a comparison of simulated and experimental MIES spectra (topmost spectrum in Fig. 1b) obtained with the DOS from Ref. [25] and by choosing appropriate rates for resonant transfer, Auger capture and Auger deexcitation. While the magnitude of Auger rates is within a factor two of those familiar from the He–metal surface interaction, the rate for resonant transfer is a factor 4 smaller than expected. According to the simulations the strong continuum emission is due to Auger capture of He+ produced by resonant ionization of He*: in the ionization process the He 2s electron tunnels into empty C_{60} states. Then, the He+ ion is neutralized by Auger capture involv-
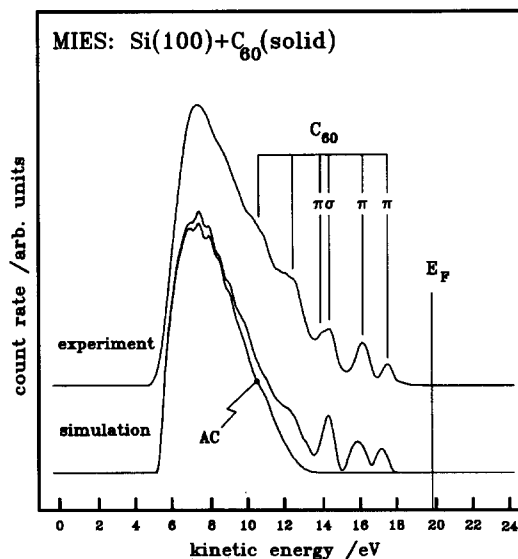
ing two C_{60} electrons. No sharp structures are produced because the spectra originate essentially from a self-convolution of the density of states of C_{60} [19,20].

In view of the relatively crude assumptions about interaction potentials and transition rates we have not attempted to improve the agreement further by considering for example the fact that He* may interact in a different way with the π and σ orbitals of C_{60}.

We noticed in Section 3 that the features from Auger deexcitation are similar, but not always identical with the features seen with UPS as far as their shape and relative intensities are concerned (see in particular the features labeled a and b in Fig. 1). The modeling of the Auger deexcitation process assumes [19,20] that it is of the exchange type, i.e. the He 2s electron is ejected. Consequently, we have neglected final state effects in the calculations of the ejection probability. Nevertheless, the MIES spectra simulated with the SDOS of Ref. [25] give rather satisfactory agreement with experiment in particular also in the region of the structures a and b. We conclude that the MIES spectra reflect rather directly the SDOS of the initially occupied states at the C_{60}. On the other hand, it has been pointed out at several occasions [11,15,24] that final state effects do drastically influence the UPS spectra. Therefore, it appears
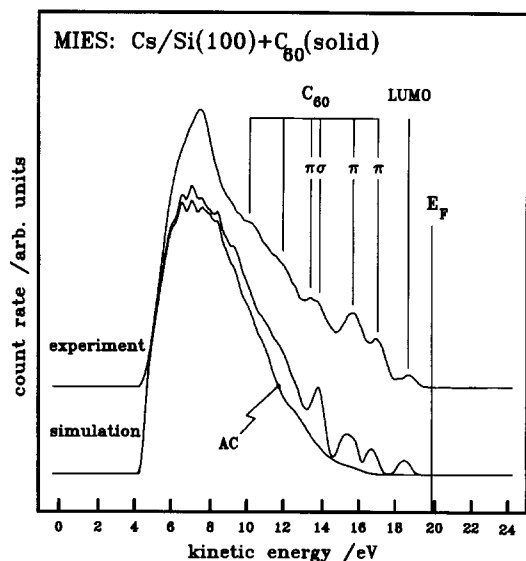
Fig. 7. Simulated and experimental MIES spectra for C_{60} on Cs/Si(100) (5th spectrum from the bottom in Fig. 3b).

that information on the SDOS of C_{60} layers can be obtained more easily from the MIES than from the UPS spectra.

Fig. 7 shows the comparison of simulation and experiment for a C_{60} film adsorbed on Si(100) saturated with Cs (at room temperature). From the fact that the Cs 5p features have just disappeared in the MIES spectra we know that the first C_{60} adlayer is complete. We have chosen the same DOS as in Fig. 6, but allowed for the population of the LUMO (HOMO–LUMO separation 1.6 eV, population ratio 5:3). A reasonable fit of the energetic position of the features from Auger deexcitation is obtained when the DOS employed for the simulations in Fig. 6 (supplemented by the occupied LUMO) is rigidly shifted to larger binding energies by about 0.8 eV. The transition rates were kept the same as for the simulations in Fig. 6. The broadening of the Auger capture contribution is caused by the lower work function of 4.4 eV (as compared to 5.5 eV in Fig. 6).

The results of the simulations suggest that there is no need to invoke collective excitation processes, such as the formation of a plasmon during the $He^* - C_{60}$ interaction, as a source for the continuous part of the MIES spectra. Clearly, other mechanisms (besides Auger capture) cannot be ruled out solely

on the basis of simulations of the spectra which employ several adjustable parameters.

4.2. C_{60}–substrate interaction

The simultaneous registration of both UPS and MIES spectra during the C_{60} exposure enables us to make the following remarks related to the C_{60}–substrate interactions.

4.2.1. C_{60}/Si(100)

The UPS spectra for C_{60}/Si(100) show a noticeable broadening of the peak from the ionization of the HOMO (h_u) during the initial stage of exposure. In addition, the structure peaking at $E_b = 6.3$ and 8.4 eV changes its shape during exposure. This is indication that there is some charge transfer from the substrate to the C_{60} adsorbate although there is no feature in the spectra which can be attributed to partial occupation of the LUMO. STM results for C_{60}/Si(100) [26] do also show little charge transfer for a defect-free surface. When the first adlayer is completed, the work function is 4.8 eV, and HOMO is centered 2.2 eV below E_F. HOMO is therefore located 7.0 eV below the vacuum level. This is close to the value of 7.2 eV for solid C_{60} [27].

4.2.2. C_{60}/SiO_2

For C_{60}/SiO_2 the energies of the two highest occupied π-type molecular orbitals fall into the substrate band gap and the peak shapes do not change much during exposure. On the other hand, the features between $E_b = 7.2$ and 5.3 eV change their intensity and shape during exposure (see in particular the UPS results). These features are resonant with states close to the valence band maximum of the substrate. The sticking coefficient on thermally oxidized SiO_2 appears to be very small: the MIES results for C_{60}/SiO_2 show emission from the substrate even after long exposure. It cannot be excluded that the adsorbate sticks only to defects at the surface. The electron affinity of surface adsorbed C_{60} is about 3.7 eV [28]. The affinity level is therefore in resonance with unoccupied defect states at the surface. This suggests that charge transfer to the adsorbate is absent. HOMO is centered around 2.3 eV below E_F. Since the surface work function is 4.8 eV, HOMO is 7.1 eV below the vacuum level.

4.2.3. Si(100) + Cs; C_{60}

For C_{60} adsorbed on Cs/Si(100) or for Cs adsorbed on C_{60}/Si(100), i.e. in cases where C_{60} can interact directly with Cs, the fullerene induced features are shifted to larger binding energies and the (former) LUMO(t_{1u}) is occupied (see also Refs. [15,11]). Moreover, the Cs 6s induced emission, labeled Cs(6s), disappears quickly in MIES, simultaneously with the onset of the t_{1u} population. These facts signal a considerable probability for the transfer of charge from the Cs 6s valence orbital into t_{1u}. The energetic positions of the observed spectral features after the completion of the first (mixed) adlayer (curve 16 from the bottom in Fig. 4b, just before Cs 5p emission is seen with MIES) is consistent with the assumption that C_{60}^- ions interact with the surface: we find a work function of about 2.9 eV, and the (former) HOMO and LUMO are centered about 2.9 and 1.1 eV, respectively, below E_F, e.g. the HOMO–LUMO separation is 1.8 eV. Thus, the states are located 5.8 and 4.0 eV below the vacuum level. It was estimated [28] that the binding energy of the additional electron at the C_{60} (occupying the former LUMO) should be 3.7 eV. The difference of the one-electron molecular eigenvalues for the former HOMO and LUMO in C_{60}^- is 1.8 eV [29]. Therefore theory predicts 5.5 eV for the HOMO's binding energy with respect to the vacuum level in surface adsorbed C_{60}^-.

When increasing the Cs exposure still further metallic-like patches appear to be formed on the first layer as judged from the appearance of the Cs(6s) feature. The C_{60} adsorbate sees probably an environment similar to that in alkali fullerides: our energetic positions are practically identical with the corresponding ones obtained for a K_6C_{60} film produced by saturating a 200 Å fullerene film with K in ultra high vacuum [30]. However we see no structure which could be attributed to emission from the (former) LUMO + 1.

5. Summary

Metastable impact electron spectroscopy (MIES) in combination with UPS (He I) was applied to study the electronic structure of C_{60} adsorbed on clean, thermally oxidized and cesiated Si(100) substrates.

The electron emission was studied during the growth of the C_{60} film starting from the uncovered substrate.

The UPS spectra of the C_{60} films agree well with those reported in previous work. We observe a strong continuous background under the discrete features from single electron ionization which, in part, may have to be attributed to autoionization after collective excitation.

The MIES spectra are dominated by strong continuous emission. Nevertheless, emission due to Auger deexcitation of He* (surface Penning ionization) is also seen, and produces spectral features similar, but not necessarily identical to UPS. MIES spectra were simulated employing a density of states available for fullerite films. The simulations agree qualitatively well with the experimental spectra. This suggests that the MIES spectra are dominated by the Auger capture process involving two electrons from the C_{60} adlayer. However, we cannot rule out contributions from other mechanisms to the continuous part of the spectra.

Charge transfer between C_{60} and the clean as well as the oxidized Si(100) surfaces is very weak. Considerable charge transfer from the Cs 6s level into the LUMO (t_{1u}) of C_{60} occurs when C_{60} interacts with the cesiated Si(100) substrate.

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