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# Synchrotron-radiation photoemission study of Ba on W(110)

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Synchrotron-radiation photoemission study of the Ba adsorption on W(110) is presented. The adsorbate $4d$ core-level spectra show sequentially the interface, surface, and the bulk components with thicknesses, as in the alkali-metals (AM) adsorption. However, in contrast to the AM adsorption, the Ba-coordinated tungsten atoms have increased the surface core-level shift to $-400$ meV, which is due to a strong interaction between the Ba $d$ and W $d$ surface states in the final state. The Ba adsorption has lowered the system work function to a minimum value of 2.02 eV, corresponding to one-third of a monolayer. Above that, Ba starts to interact with the charge underneath the W surface layer. As a result, a bulk valence state originated from that region shifts toward higher binding energy, and a component, shifted $+107$ meV, appears in the W $4f$ core-level spectra. [S0163-1829(98)11231-6]

## INTRODUCTION

A universal observation of the alkali-metals (AM) deposited on metallic substrates as Al and W is a clear manifestation of three components in core-level photoemission spectra and lowers the system work function. The three components are associated with the layers from surface, bulk, and interface.[1–4] The first two components show up at a fixed energy upon the completion of one monolayer (ML), while the interface component appears first and shifts gradually toward smaller binding energies with thickness. Since the interface component is still visible when the thickness of the AM overlayer is over 2 ML, the formation of clusters or islands is then assumed. The work-function lowering has long been modeled as ionic interaction. However, there comes a consensus that the AM adsorbate is actually polarized,[2,5–8] meaning that the charge remains in the adatoms. Detailed core-level photoemission studies of the AM adsorbate and of the substrate illustrate clearly the retention of the $ns$ electron in it.[2,6,7]

The above description of the AM-adsorbate behavior might suggest that the interface is abrupt. In the Na/Al(111) system,[9,10] however, there is an intermixing that occurred at room temperature (RT), meaning that the Na adatoms have substituted the surface Al atoms. Specifically, this phenomenon occurs at a $\sqrt{3}\times\sqrt{3}$ ordered structure, which corresponds to one-third of a monolayer. Upon further coverage, the intermixing gets even stronger so that multilayer surface alloys are obtained. However, the layerwise resolution of the interface, bulk, and surface components still maintains at 100 K of temperature.[1] Needless to say, the AM adsorption on a metallic substrate is far from a simple system.

Compared to quite a few studies on the AM adsorption, little effort has been made to the alkaline-metals adsorption. Thus, in this paper, we present the synchrotron-radiation photoemission study of the Ba adsorption on W(110), assisted by low-energy electron diffraction (LEED) techniques. The divalent-Ba adsorption in some parts behaves similarly as the monovalent-AM adsorption. For example, three distinct components associated with bulk, surface, and interface layers are also found in the Ba core-level photoemission spectra. However, some differences exist. For example, we find a component in the W $4f$ core-level spectra, having greater surface core-level shift (SCLS) than the surface component. This component is absent in the AM adsorption.[2,5–8] The Ba adsorption also causes a minimal surface-atom displacement above a threshold thickness corresponding to the work-function minimum ($\phi$).

## EXPERIMENT

Photoemission experiments were performed at the Synchrotron Radiation Research Center in Hsinchu, Taiwan, R. O. C. The details can be found elsewhere.[11] In short, photoelectrons were collected via a 125-mm hemispherical analyzer (OMICRON electron spectroscopy, Inc.) in an UHV chamber with a base pressure better than $3\times10^{-11}$ Torr. A clean W(110) surface was annealed a few times at 1200 °C under $1\times10^{-7}$ Torr oxygen atmosphere for 1 h, followed by repeatedly flashing at 2200 °C lasting for a few seconds. The thoroughly degassed Ba getters (SAES, Inc.) were controlled to allow depositions under $1.2\times10^{-10}$ Torr. Each energy distribution curve (EDC) with various Ba coverage was collected from a freshly made interface, and the presented ones, taken at normal emission and normalized to the mesh current, were referred to their changes in work function as well as the coverage. 1 ML in the present study is defined as the saturation coverage, which shows an fcc(111) adlayer pattern.

## RESULTS

Figure 1 exhibits the LEED patterns for (a) clean, (b) 0.5 ML, and (c) 1.0 ML of Ba deposited on W(110). As can be seen in Fig. 1(a), the clean W(110) surface shows a sharp, intense $(1\times1)$ LEED pattern with a high contrast in background. Upon 0.5-ML Ba adsorption, the background intensity increases, and the $(1\times1)$ spots get blurred but remain bright, indicating the formation of a pseudomorphic Ba adlayer on W(110). At 1 ML, the LEED pattern changes drastically with the appearance of the characteristic doublets in the [001] direction. The six extra bright spots around the (00)

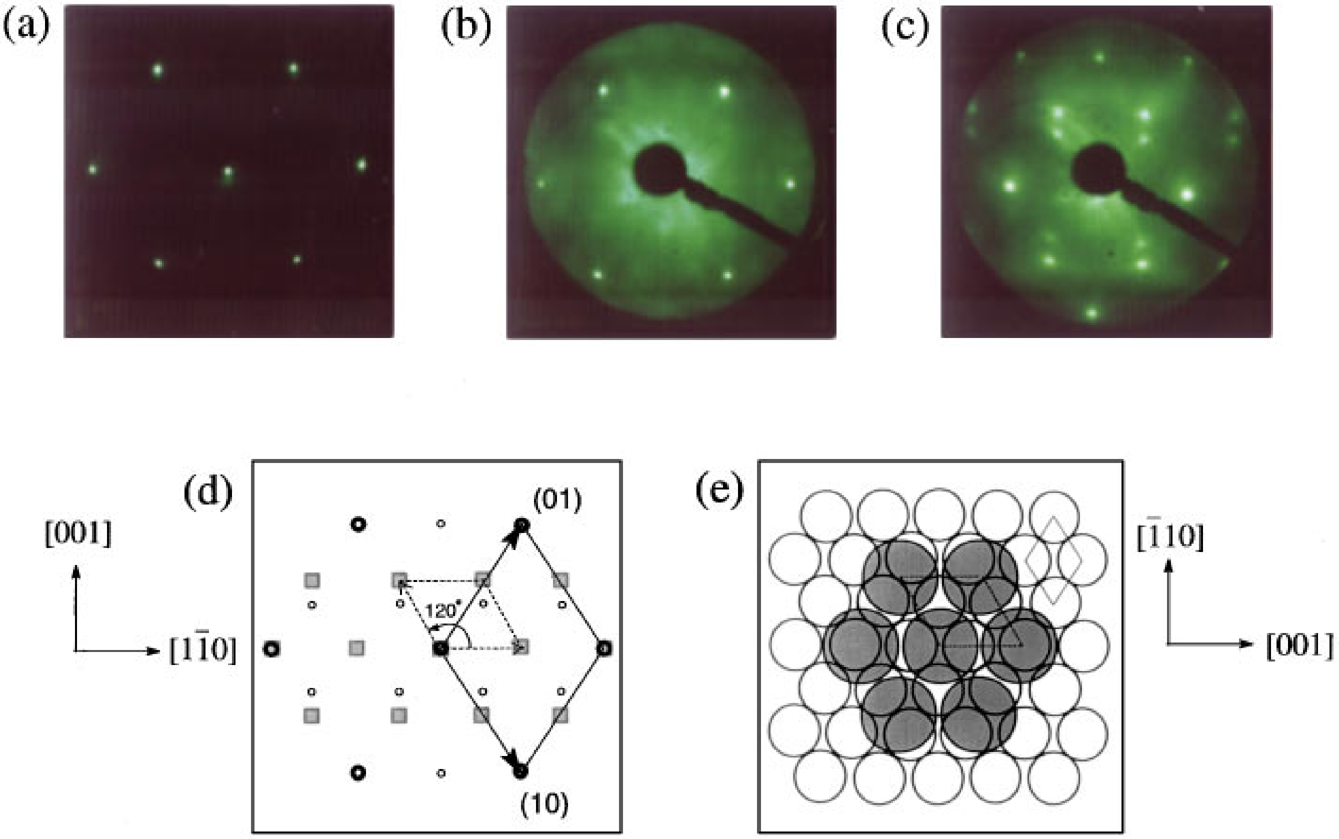

FIG. 1. (Color) (a)–(c) show the LEED patterns of Ba on W(110) at RT. (a) The clean W(110) surface, $E_p = 64$ eV. (b) 0.5 ML Ba, $E_p = 76$ eV. (c) 1 ML Ba, $E_p = 38$ eV, indicating the formation of a close-packed fcc(111). (d) The schematic drawing corresponding to (c). The large-solid circles and the hatched squares denote the W and Ba atoms, respectively. The small-solid circles denote the multiple scattered satellites. (e) The atomic arrangement of ML Ba on W(110). The W and Ba atoms with exact relative sizes are plotted in open and hatched circles, respectively.

beam are the diffraction arisen from the hexagonal Ba overlayer of fcc(111) face.[12] A schematic drawing of the reciprocal space at 1 ML is shown in Fig. 1(d). The large circles and squares denote the LEED spot positions for W and Ba atoms, respectively. The small circles along the [001] direction are satellites that are due to the multiple scattering between the W substrate and Ba monolayer. The high brightness of the spots associated with the barium adatoms indicates their good long-range ordering. Furthermore, the preservation of the sharp spots associated with the tungsten atoms is manifest that the substrate lattice structure has undergone little change upon Ba adsorption. In other words, no alloying has occurred. The later core-level photoemission data support this statement. A similar pattern has been reported in 1-ML Ba on W(110) (Ref. 13) and 0.9-ML Cs on W(110),[14–16] both at 77 K. The atomic arrangement in the real space is drawn in Fig. 1(e). As shown in the figure, the Ba monolayer forms a close-packed hexagonal overlayer on W(110) with a Nishiyama-Wassermann mode.[17] The Ba overlayer is oriented with the W surface in the direction of $[1\bar{1}0]_{\mathrm{fcc}} \| [001]_{\mathrm{bcc}}$. That is to say, the Ba adatoms grow epitaxially on the W(110) surface.

Upon Ba adsorption, the work function is lowered to 2.02 eV, corresponding to one-third of a monolayer. The change in work function in the Ba adsorption on W(110) is shown in Fig. 2. The behavior of $\Delta\phi$ is similar to the case of the AM adsorbate, a rapid decrease in $\Delta\phi$ to a maximum value followed by a slight rise and a plateau afterwards.

Figure 3 displays the evolution of the valence-band spectra of Ba on W(110) taken in normal emission. The detailed discussion of the valence-band EDC's can be found elsewhere.[11] For the sake of completeness, we, in the present

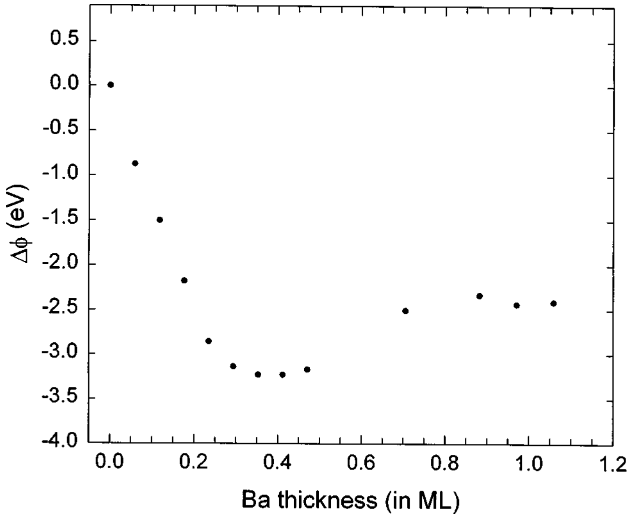

FIG. 2. The change in the work function of Ba on W(110).

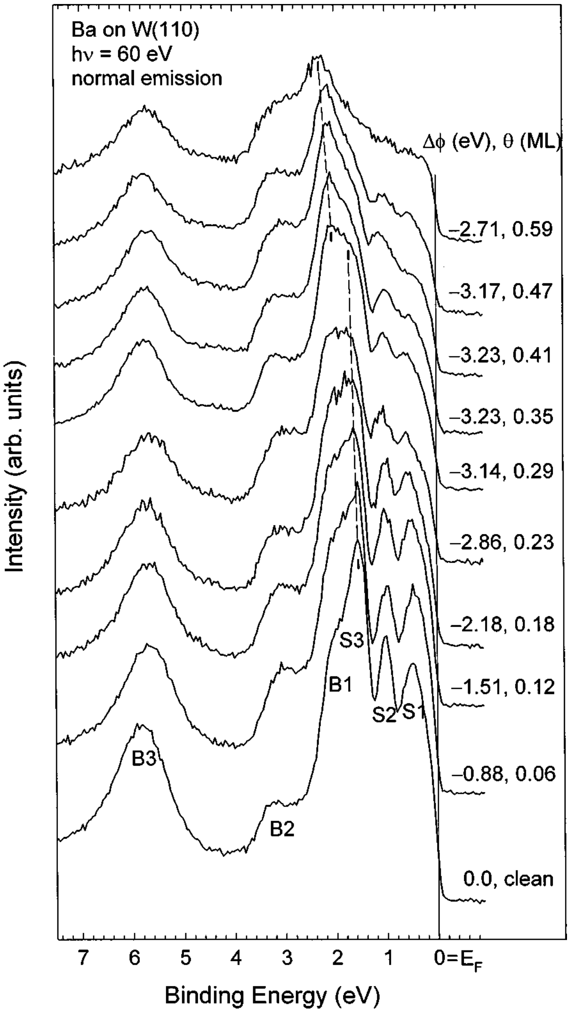

FIG. 3. Valence-band spectra of Ba on W(110). Symbols $S1$, $S2$, and $S3$ are surface states, and $B1$ and $B2$ are bulk states.

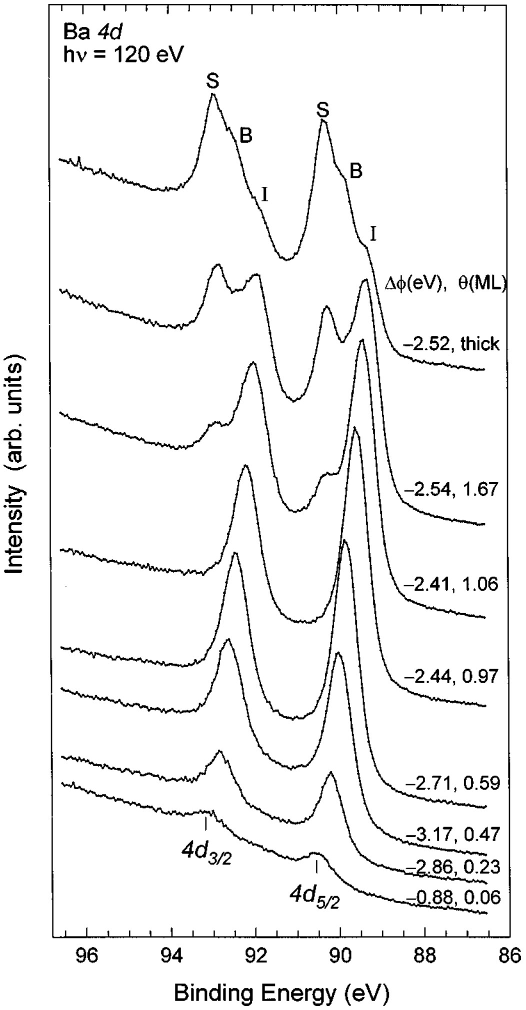

FIG. 4. Ba $4d$ core-level spectra of Ba on W(110). Components $I$, $S$, and $B$ are from atoms in the interface, surface, and bulk layers, respectively.

paper, include them with a 60-eV photon energy. In short, three surface states at 0.41 ($S1$), 0.95 ($S2$), and 1.41 ($S3$) eV, and three bulk states at 2.0 ($B1$), 3.27 ($B2$), and 5.8 ($B3$) eV are found for the uncovered surface. Upon Ba adsorption, the Fermi edge remains sharp and strong. All the surfaces states attenuate gradually in intensity with coverage and are well quenched at $\Delta\phi = -2.71$ eV, corresponding to 0.59 ML. Among the three surface states, the Ba adsorption affected the most on $S3$, where the line width is broadened the most and the downward line shift is the greatest, about 220 meV at $\phi_{\min}$. The only noticeable features above $\Delta\phi = -2.71$ eV are narrow Fermi edge, small $S2$, $B1$, and $B2$. These features persist even to the monolayer coverage.

As can be seen in Fig. 3, the $B1$ state has unexpectedly revealed an energy shift upon Ba adsorption, while the $B2$ state has not. However, the shift does not happen until $\phi_{\min}$, after which $B1$ starts to move gradually toward higher binding energy by 260 meV at $\Delta\phi = -2.71$ eV (or 0.59 ML). Hence, the assignment of $B1$ as mere bulk emission is then questioned, even though it truly shows dispersion with photon energies.[18] Nevertheless, it is possible that the $B1$ state might originate from electrons embedded between the top surface and the second layers. The later W $4f$ core-level spectra support this statement.

Figure 4 demonstrates the representative EDC's of the Ba $4d$ core-level spectra with coverage. The excitation photon energy is 120 eV. As shown in Fig. 4, three components are clearly seen in the highest-coverage spectrum at binding energies of 89.25, 89.80, and 90.30 eV, labeled as $I$, $B$, and $S$, respectively. The interface component $I$ was initiated at 90.6 eV corresponding to a thickness of 0.06 ML. Upon further coverage, it shifts gradually toward lower binding energies until the completion of 1 ML, where a maximum intensity is reached. Upon further adsorption, a second component, $S$, commences to appear and grows stronger in line intensity with a fixed line position with coverage. In the uppermost spectrum of Fig. 4, the $B$ component shows up as a shoulder on the lower-binding-energy side of the $S$ component. The sequence of the appearance of components $I$, $S$, and $B$ follows exactly the same as the AM adsorption on a W(110) surface,[2] and an Al(111) surface[1] as well. Moreover, the binding energies of the $S$ and $B$ components are the same as that reported in Ba on Al(111).[19] However, the interface component is absent in the Ba/Al(111) system.[19]

The representative EDC's of the W $4f_{7/2}$ cores excited by a 70-eV photon energy with the Ba thicknesses below 1 ML are displayed in Fig. 5. Coverage higher than that exhibits little changes on the line shape (not shown). As can be seen

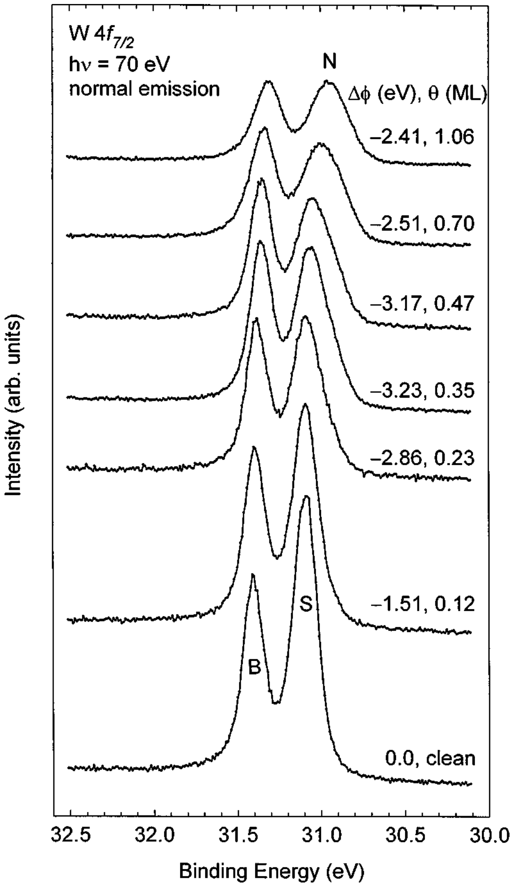

FIG. 5. W $4f_{7/2}$ core-level spectra of Ba on W(110). Symbols *B* and *S* denote bulk and surface emission, respectively. The *N* component is the Ba-induced component.

in Fig. 5, the uncovered W $4f_{7/2}$ cores show strong surface emission. In a separate report, it is demonstrated that a minimal oxygen residue has a strong impact on the evolution of Ba-covered W $4f$ core-level spectra.[18] Upon Ba adsorption, clean surface emission reduces gradually in intensity. In the meantime, an adsorbate-induced component *N* starts to develop as a shoulder structure on the lower-binding-energy side of the clean-surface peak, and gains strength gradually with increasing coverage. The appearance of this structure was not found in Cs on W(110),[2] although the valence-band EDC's of both Ba on W(110) and Cs on W(110) exhibit similar spectral changes.[11] As shown in Fig. 5, the maximum height of surface-related emission falls gradually below that of bulk emission, with the least magnitude at half of a monolayer. At 1.06 ML, the surface-derived emission has regained the strength and exhibited the same height as bulk emission, meaning that the Ba adatoms have covered entirely the W surface.

## DISCUSSION

Previous Cs adsorption on $5d$ metals[11,20,21] and theoretical calculations[5] have concluded that there is a formation of a polarized covalent bonding between the Cs $s$ and the substrate $d_{z^2}$-like surface states. As to the Ba/W surface, the calculations were only performed on 1-ML Ba on W(100) in a $c(2\times 2)$ overlayer structure by Hemstreet and Chubb (HC) (Ref. 22) and Lamouri, Müller, and Krainsky,[23] who employed the all-electron full-potential linearized augmented-plane-waves method and the embedded-cluster-model method, respectively. These calculations have found that it is the Ba $d$ states that interact heavily with the W $d$ surface states. This $d$-$d$ interaction results in the redistribution of charge, which is drawn from the adlayer and substrate into the interfacial region. As a result, Fermi emission becomes an admixture of the W and Ba states, with the loss (enhancement) of $d$ character in the former (latter). The angle-resolved inverse photoemission work[24] further confirmed the calculation.

The apparent agreements of the theory and experiments let one conclude that on a W(100) surface, the responsible bonding orbital for Cs is $s$ like, while for Ba is $d$ like. These differences in bonding orbital have been attributed to their different equilibrium heights, being 2.48 Å for Ba and 2.75 $\pm 0.15$ Å for Cs. It is then clear that Ba adatoms being close to the W surface enhance the Ba($d$)-W($d$) interaction, while the weaker Cs($s$)-W($d$) interaction is due to Cs adatoms positioned farther away from the surface. It is worth mentioning that the Cs $d$ state could involve in the interaction if the optimal height decreases.[15] In fact, the hybridized Cs($d$)-W($d$) state was found just a few tenths of an eV above the Fermi level.[5]

To the best of our knowledge, there have been no reports of theoretical calculations on the Ba/W(110) system, nor a valence-band photoemission work of Ba on any W face. Nevertheless, the valence-band spectra in Fig. 3 have shown an agreement with the HC calculation, which predicts that the Ba adsorption affects the most low-lying $S3$ surface state over other surface states. Two conclusions are thus derived. On the one hand, the behavior of the Ba adsorbate on tungsten is independent of the surface structures. On the other hand, the nature of the Ba bonding state with W(110) is $d$ like and the surface states near $E_F$ acquire a significant admixture of Ba $d$ character. Since the HC calculation was performed on a 1-ML Ba surface where the adatoms occupy the four-fold hollow sites in a $c(2\times 2)$ configuration, we then can assume similar occupation sites for Ba on W(110). As can be seen in Fig. 1(e), the LEED pattern illustrates that the 1-ML Ba structure is actually an incommensurate hexagonal close-packed fcc(111) surface in registry with the tungsten substrate along [001] direction. In this incommensurate structure, the mismatch of the hexagonal lattice between the adlayer and substrate renders the Ba adatoms positioned at inequivalent sites on the W(110) surface. If the highest-coordinated two-fold long-bridge sites are occupied to fulfill the $C_{2v}$ symmetry manifested in LEED, then the Ba adatoms should occupy some of the short-bridge sites as well as the atop sites. With this arrangement, the hexagonal pattern of the 1-ML Ba and the multiple-scattered satellites in the [001] direction can be achieved.

The SCLS of Ba was reported to be $+0.50$ eV in the Ba/Al(111) system.[19] This magnitude is in good agreement with the SCLS of the *S* component in Fig. 4. As to the interface component, its SCLS moves progressively from a positive ($+0.8$ eV corresponding to 0.06 ML) to a negative ($-0.55$ eV corresponding to 1 ML) value. With the trend of decreasing binding energy with increasing coverage, the binding energy of this component should be even greater at lower coverage.

Barium has a unique property that is not found in other elements; that is, the photoexcited oxidization state always appears in a *lower* binding energy than the clean state.[19,25] The phenomenon is attributed to the admixture of the $5d$ orbital that lies just above the Fermi level in the conduction band. Moreover, the loss of the $6s^2$ electrons in Ba compounds increases the negative shift of the oxidization states since the empty $5d$ states are now energetically favorable to be filled. The key point here is that the filling of the *d* state, either intra-atomically or interatomically, increases the effectiveness of the final-state screening. Thus, applying this unique property of Ba to the present system, one expects that an increased $6s$-$5d$ admixture or a charge transfer from the tungsten substrate will result in an upward shift of the core-level binding energy. As shown in Fig. 4, the binding energy of the interface component is high in thin thickness, clearly indicating that the $6s^2$ electrons are mostly retained at low coverage. As the coverage becomes thicker, the upward line shift illustrates that the $5d$ band is now partially filled. Therefore, the decrease in the binding energy of the interface component with coverage is a direct indication of a gradual increase in the *d* occupancy of the Ba overlayer. The predominance of the *d* charge in the final-state screening can also explain the observation in the AM adsorbates where the magnitude of the negative shift of the interface component is greater in the later alkalis.[3] This is because their *d* state lies closer to the Fermi level,[4] thus making it play a stronger role in the participation of the screening in the final state.

We have used a nonlinear curve-fitting routine to analyze the W $4f$ core-level spectra in Fig. 5, and the selective fit is presented in Fig. 6. In a fit, the line shape is generated by a convolution of the Gaussian function with the Doniach-Šunjić function broadened by a lifetime function. The background function is represented by a power-law form. On a clean surface, the lifetime width ($\Gamma_L$), excess Gaussian width ($\Gamma_G$), and an asymmetric index ($\alpha$) for the bulk (surface) component are 60 (81) meV, 66 (75) meV, and 0.038 (0.087), respectively. The SCLS is $-320\pm1$ meV. All these values compare comfortably with the report of Riffe, Wertheim, and Citrin,[26] although the surface $\alpha$ is a bit higher. To fit a spectrum with a given Ba coverage, we implant a few constraints stated as follows. For the bulk and surface components, the lifetime widths and $\alpha$'s are fixed at the values of those in the clean surface. As to the *N* component that is originated from the W surface atoms coordinated with Ba, we let its $\Gamma_L$ and $\alpha$ fixed at the values of saturation, where only one shifted component is observed, with the magnitudes of 53 meV and 0.050, respectively. Therefore, the total adjustable parameters for a Ba-covered spectrum are 13.

The fitted results in Fig. 6 reveal clearly a few phenomena. First, the binding energy of the bulk component gradually decreases with increasing coverage, from 31.40 eV in a clean surface to 31.31 eV at 1.06 ML. Its excess width has increased to 134 meV, almost twice as wide as that on the clean surface. Second, the SCLS at 0.70 ML reduces to $-279$ meV, a 42-meV reduction from the clean surface. Here, the excess width of the surface component has widened to 105 meV. The decrease of the SCLS is attributed as a slight reduction in charge associated with the surface atoms. Third, the binding energy of the *N* component is 30.99 eV below $\phi_{\min}$, and decreases to 30.92 eV above that. The SCLS of the *N* component is then in average of $-400$ meV. The excess width of component *N* is 178 meV at 0.12 ML, but it increases to 215 meV at the saturation coverage.

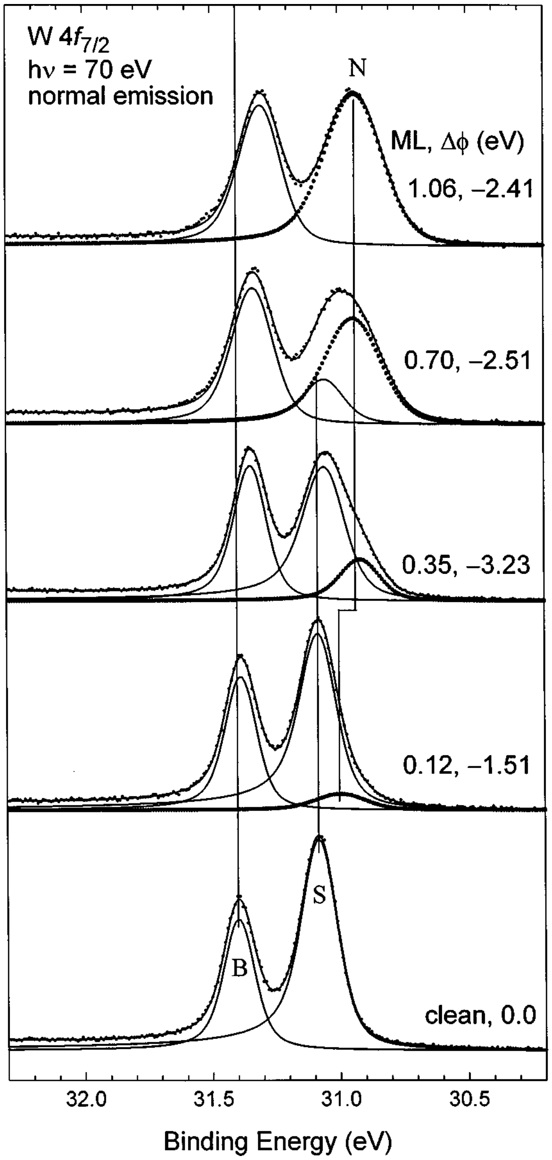

FIG. 6. Curve-fitting analysis to the W $4f_{7/2}$ core-level spectra.

The facts that the intensity of the surface component decreases gradually to zero at the saturation coverage and only one induced component is observed in the submonolayer region suggest that each coordinated surface atom has similar chemical environment. With this and the existence of only one interface component of the Ba $4d$ cores, the Ba adlayer is grown in a layerwise fashion without forming clusters or islands.

Previously, the AM adsorption on W(110) induced a negligible surface core-level shift.[2,6,7] From this, a noncharge transfer of the monovalent AM was derived. In other words, having not gained extra charge from the AM adsorbate, the surface atoms appear a negligible shift from the bulk component. It is apparent that the initial-state effect dominates this phenomenon. However, the present study indicates that the disappearance of an interface-derived component[2,6,7] is possible from nonoccupancy of the *d* states in the final state, whose energies lie high above the Fermi level.

The SCLS of the *N* component is greater than that of component *S*, meaning that the former is better screened.[27] The effective screening in the final state also renders the bulk component a small but noticeable upward shift. This shift is hard to comprehend in the framework of the initial-state effect, which would lead one to speculate that the adsorbate charge had penetrated into the bulk. As to the line broadening, it is a result of the coupling of the core-hole excitation to a longitudinal Debye phonon function.[28–30] At temperatures higher than the Debye temperature ($\Theta_D$), this electron-phonon coupling increases linearly with the Fermi energy and with the inverse of $\sqrt{\Theta_D}$,[28–30] which is then proportional to the square root of the electron density. Thus, the increased broadening of the induced component is due to this increase in charge density in the interfacial region, as illustrated in the HC calculation. The electronic-phonon coupling effect can also explain satisfactorily the increased Gaussian width of the bulk component at the saturation coverage. Since most of the Ba adatoms are adsorbed on the bridge sites of W(110) surface at 1 ML, the broad linewidth of the *N* component is thus mainly an electronic effect, not a structural effect.

In Fig. 6, one might notice that the fit is unsatisfactory for thick curves. Figure 7(a) displays a fit to the 0.7-ML spectrum, using the three-component model function. As can be seen in Fig. 7(a), the residual curve exhibits an unresolved structure on the high-binding-energy side of the bulk component. In a revisited analysis, we found that the model function with three components works fine for the spectra of thicknesses below $\phi_{\mathrm{min}}$. Above that, a fourth component must be added in the model function for a better fit. Figure 7(b) then shows the result of a fit with the four-component model function. In this fit, we add only $\Gamma_G$, line position, and intensity to the model function for the new structure. The lifetime width and $\alpha$ are fixed with respect to the bulk component. As shown in Fig. 7(b), this fourth component, *A*, removes the structural fluctuation in the residual curve, and improves $\chi^2$, from 2.21 to 1.33. The core-level shift of the *A* component is +107 meV, and its excess Gaussian width is 175 meV. The excess width of the bulk component now reduces to 109 meV.

There have been reports of the structural change on the W(110) surface upon Re (Ref. 31) and H (Ref. 32) adsorption. Consequently, the surface $4f$ core levels have shown a gradual integration with the bulk $4f$ core levels. In the Ba/W system, however, the absence of this integration indicates that the interface of Ba and W is abrupt without undergoing a drastic structural change, as in the case of Gd on W(110).[33] Nevertheless, some miniscule atomic displacement cannot be excluded. This displacement occurs above a thickness corresponding to the work-function minimum, and results in a shift of the *B*1 bulk state toward higher binding energy as well as the appearance of a positively shifted component in W $4f$ core-level spectra. Nevertheless, this postulation needs further theoretical justification.

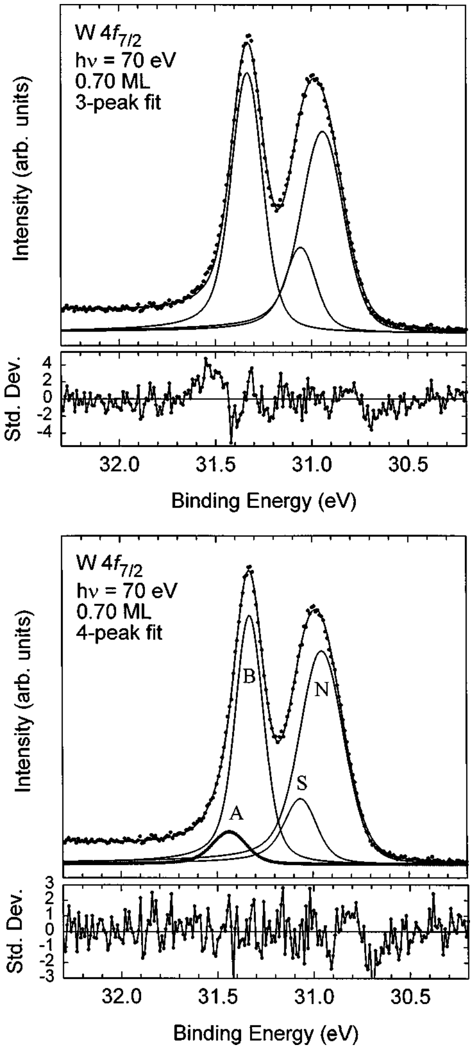

FIG. 7. 0.7 ML Ba on W(110). (a) Three-peak fit for the W $4f_{7/2}$ core level, (b) four-peak fit for the W $4f_{7/2}$ core level.

## SUMMARY

We have studied the Ba adsorption on an atomically clean W(110) surface, mainly using synchrotron-radiation photoemission as a probe. The core levels of the alkaline adsorbate manifest a similar evolution as the AM adsorbates; that is, an interface component appears first, followed sequentially by surface and bulk components. However, in contrast to the AM adsorbates, the Ba-contacted surface W atoms have a new SCLS of about −400 meV. Further, the Ba adsorption results in a bulklike component at +107 mV when the thickness is greater than $\frac{1}{3}$ ML. We postulate that the W surface atoms have displaced slightly from their clean position so that the Ba *s* electrons interact the charge right underneath the topmost surface. This disturbance in charge has concurrently caused a downward shift of the bulk *B*1 state. The attribution of the *s* character responsible for the interaction is based on the fact of the parallel behavior of the *B*1 state in Ba on W(110) and Cs on W(110).

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