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Surface band structure of Al(1 0 0) studied with high-resolution angle-resolved photoelectron spectroscopy

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ABSTRACT

From an examination of the Al(1 0 0) surface band structure with high-resolution angle-resolved photoelectron spectra, we identified three surface states. Features in the surface band structure predicted theoretically were confirmed experimentally, including the dispersion of the surface state within the narrow band gap centered at $\bar{X}$, an avoided crossing between two surface states along $\bar{\Gamma}\bar{X}$, and the dispersion of the surface state within the symmetry gap along $\bar{\Gamma}\bar{M}$. The electron–phonon coupling strength of the surface state at $\bar{\Gamma}$ was determined. Our results indicate that there is no thermally induced defect on Al(1 0 0) from 90 to 420 K. Our photoemission data serve as reference for future investigation and motivate re-examination of many systems with contemporary photoemission instruments.

1. Introduction

The surface of a single crystal of aluminium, a trivalent nearly free-electron-like metal, has long been considered a model system to test the validity of diverse theoretical and experimental approaches. Among many surface properties, the surface states of aluminium have attracted much interest since they were reported experimentally in 1978 [1,2]. The results from these early measurements of angle-resolved photoemission showed that the surface states of aluminium exist both inside and outside the projected bulk band gaps. Numerous theoretical investigations explored this behavior; an extensive list is found in Ref. [3]. Surface states are generally agreed to exist in not only the absolute band gap but also "the symmetry gap" [4,5] (also called "filled band gap" [2] and the "partial Bragg reflection bulk energy gap" [6] by various authors). The complete surface band structures of aluminium were reported in the studies based on the geometry of a semi-infinite crystal [3,4].

In contrast to the theoretical results, the experimental data for aluminium surface band structures are far from complete. In the case of Al(1 0 0) (cf. Fig. 6 in Ref. [3] and Fig. 8 in Ref. [4] for the results of calculations), several authors reported the dispersion of the surface state near $\bar{\Gamma}$ [1,2,7,8]; the surface state near $\bar{X}$ was observed, but only its binding energy was reported [7]. Many features of the surface band structure predicted theoretically have not been observed, such as the dispersion of the surface state within the narrow band gap near $\bar{X}$, the surface resonance and the avoided crossing between the two surface states along $\bar{\Gamma}\bar{X}$, and the surface state within the symmetry gap along $\bar{\Gamma}\bar{M}$. This scarcity of experimental data resulted partly from the difficulty of measuring angle-resolved photoemission in an off-normal geometry with traditional electron energy analyzers. In recent photoemission experiments, electron energy analyzers were equipped with a two-dimensional channel plate, but predicted features in the surface band structure of Al(1 0 0) were still not observed [9,10]. A common practice to evaluate a theoretical approach involves a comparison of its results with experimental data. The failure to observe many theoretically predicted features in experiments casts doubt on the validity of the theoretical works on the Al(1 0 0) surface.

To address this discrepancy, we re-examined the Al(1 0 0) surface with high-resolution angle-resolved photoelectron spectroscopy (ARPES). With the improved angular resolution and sampling accuracy, we measured the photoemission along the high-symmetry lines in the surface Brillouin zone of Al(1 0 0), and identified several theoretically predicted features in the surface band structure. Our results not only confirm the predictions from

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preceding theoretical works but also provide experimental data of high quality as reference for future investigations.

2. Experiment

The experiments were performed at an end station attached to the ultra-high-resolution and high-flux U9 cylindrical-grating beamline (BL21B) at National Synchrotron Radiation Research Center, Taiwan. An Al(1 0 0) single crystal (diameter 1 cm, miscut <0.1°) was mounted on a manipulator. The sample temperature, variable from 60 K to 1000 K, was measured with a thermocouple junction (type E) mounted beside the sample. The Al(1 0 0) surface was cleaned with 1.5-kV Ar-ion sputtering and annealing at 450 °C in repeated cycles until a sharp p(1 × 1) low-energy electron diffraction (LEED) pattern was obtained. Photoemission was measured with the photon energy varied from 21 to 54 eV. The distribution of photoelectron energy was recorded with an electron energy analyzer (Scienta SES200) equipped with a two-dimensional channel plate and a charge-coupled-device camera, allowing 96 spectra at various emission angles to be collected concurrently with angular resolution 0.125°. The axis of the acceptance cone of the analyzer (*A* axis) and the incident axis of the photon beam (*P* axis) were fixed at angle 45° to each other. The polarization of the incident photons and the angular dispersion plane of the analyzer both lay in the plane spanned by the *A* and *P* axes. To acquire the photoemission spectra over a wide range of $k_{||}$ (the component of the wave vector of photoelectrons parallel to the surface), we combined the data of several consecutive measurements as a simple linear combination in the region of overlap without further intensity normalization. The estimated resolutions are less than 30 meV for kinetic energy and less than 0.01 Å^{-1} for $k_{||}$.

3. Results and discussion

The photoemission from Al(1 0 0) along the high-symmetry lines, $\bar{\Gamma}\bar{X}$ and $\bar{\Gamma}\bar{M}$, in the surface Brillouin zone was measured with many photon energies. Fig. 1 displays representative results measured with photon energies 54 eV [Fig. 1(a) and (b)] and 45 eV [Fig. 1(c) and (d)]; the photoemission along $\bar{\Gamma}\bar{X}$ with photon energy 50 eV is shown in Fig. 3(a). Plotted against the binding energy and $k_{||}$, the photoemission intensity is normalized independently in each figure and illustrated with varied color; white marks the greatest and black the least intensity. Fig. 1(b) covers a range of binding energy wider than the others. The regions enclosed with green dashed lines indicate the projected bulk band gap. Many features are readily identified with lines of lighter colors. The origins of these features might be either surface- or bulk-related; they are discerned on comparing the photoemission measured with varied photon energy. The binding energy of surface-related features remains constant whereas the binding energy of the bulk-related features might vary with the photon energy [7]. The photoemission intensity of an electronic state can be significantly modulated by several factors, such as the photon-energy dependent photoionization cross section and the polarization of the incident photons. To identify the surface states properly, one must measure the photoemission with varied photon energies.

Three surface states are identified and denoted as S_1, S_2, and S_3 in Fig. 1. The dispersions of these surface states were determined by analyzing each curve of energy distribution. Plotted as the black dots in Fig. 2, the dispersions are nearly free-electron-like, and their effective masses are determined on fitting them to second-order polynomial functions; the fitted results are shown as the yellow solid lines in Fig. 2. In Fig. 2(b), the dispersions are modulated because of the avoided crossing between the dispersions; only the data close to $\bar{\Gamma}$ (for S_1) and $\bar{X}$ (for S_2) are included in the

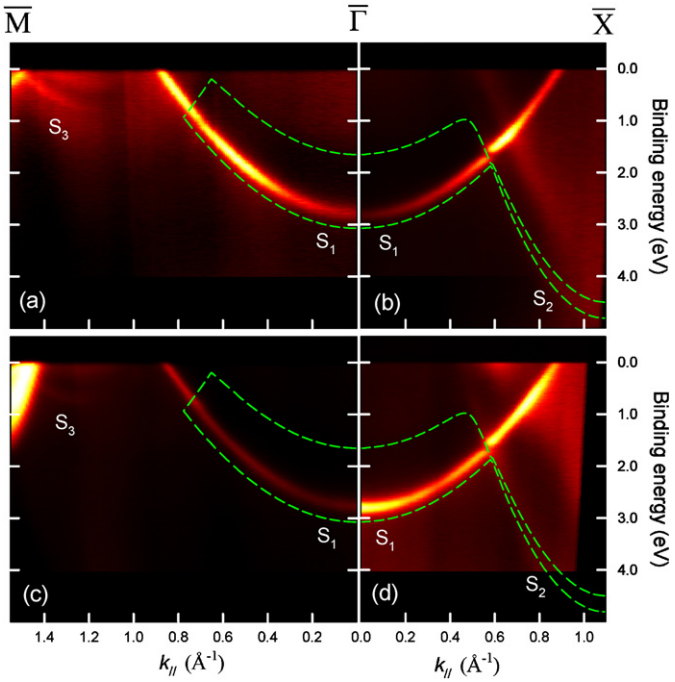

Fig. 1. Intensity of photoemission from Al(1 0 0) (a) along $\bar{\Gamma}\bar{M}$ with photon energy 54 eV; (b) $\bar{\Gamma}\bar{X}$, 54 eV; (c) $\bar{\Gamma}\bar{M}$, 45 eV; (d) $\bar{\Gamma}\bar{X}$, 45 eV. S_1, S_2 and S_3 label the surface states. The regions enclosed with green dashed lines are the bulk projected band gap. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

fitting. The detailed dispersions of the Al(1 0 0) surface states were reported in the previous theoretical studies [3,4]; the result published in Fig. 8 of Ref. [4] is plotted as the blue dashed lines in Fig. 2 for comparison. Our photoemission results agree qualitatively with this theoretical result with the noticeable deviation in the binding energies.

3.1. Surface band structure along $\bar{\Gamma}\bar{X}$

Figs. 1(b), (d), 2(b), and 3(a) show the photoemission results along $\bar{\Gamma}\bar{X}$. Two surface states, S_1 and S_2, are identified. The binding energy of the broad feature on the upper right side varies with photon energy, demonstrating its bulk-related nature. According to preceding works, S_1 is centered at $\bar{\Gamma}$ and follows a nearly

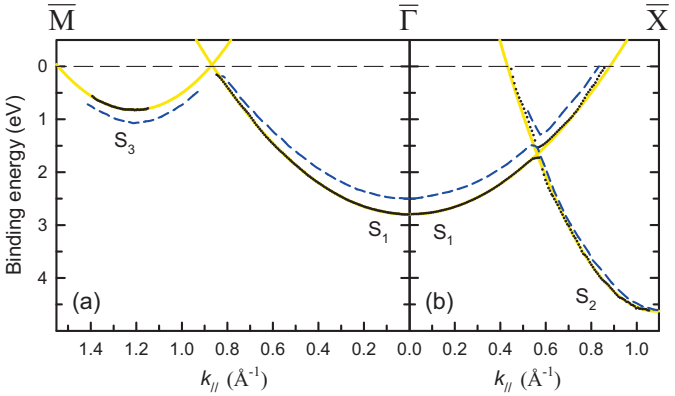

Fig. 2. The dispersion of the Al(1 0 0) surface states, denoted as S_1, S_2 and S_3, along (a) $\bar{\Gamma}\bar{M}$ and (b) $\bar{\Gamma}\bar{X}$. The black dots are the results from photoemission measurements. The yellow solid lines are the results from fitting the dispersions to second-order polynomial functions. The blue dashed lines are the theoretical results reproduced from Fig. 8 in Ref. [4]. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)