Atomic orbital character of Ni-O surface complex studied by two-dimensional photoelectron spectroscopy

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1. Introduction

Stepped surface of metals have regular arrays of atomic rows at step edges. These steps must have significant influences on the surface electronic states on the stepped surfaces. For example, one-dimensional electronic states have been found on the stepped surface of Ni(755) [= 6(111) × (100)] [1]. Utilizing a stepped surface as a substrate, nano-structures have also been fabricated, e.g., Co nanocluster on Cu(755) [2]. Recently we found the formation of one-dimensional Ni-O surface complex along the step edges on Ni(755) stepped surfaces by oxygen adsorption [3]. In order to clarify the electronic structure of the Ni-O surface complex, we have performed two-dimensional photoelectron spectroscopy (2D-PES) measurements which enable us to obtain a constant energy surface at once and hence to know the dimensionality and the bonding orbital character from the photoelectron intensity angular distribution (PIAD).

2. Experimental

The experiment was performed at the linearly polarized soft x-ray beamline BL-7 equipped with a two-dimensional display-type spherical mirror analyzer [4] at SR center, Ritsumeikan University [5]. Surface cleanliness and oxygen adsorption at steps were confirmed by low energy electron diffraction and Auger electron spectroscopy. Photon energy for 2D-PES was set to 40 eV and the total energy resolution was set to about 0.4 eV. The PIAD of this experiment was collected by energy window of 0.1 eV. Typical acquisition time for one PIAD was 10 sec. The angular resolution was about 1°.

3. Results and Discussion

Figure 1(a) shows the angle-integrated energy distribution curves measured on the clean and the oxygen adsorbed surfaces of Ni(755). By oxygen adsorption, new electronic state emerges around the binding energy of 6 eV. However, the PIADs around oxygen-derived

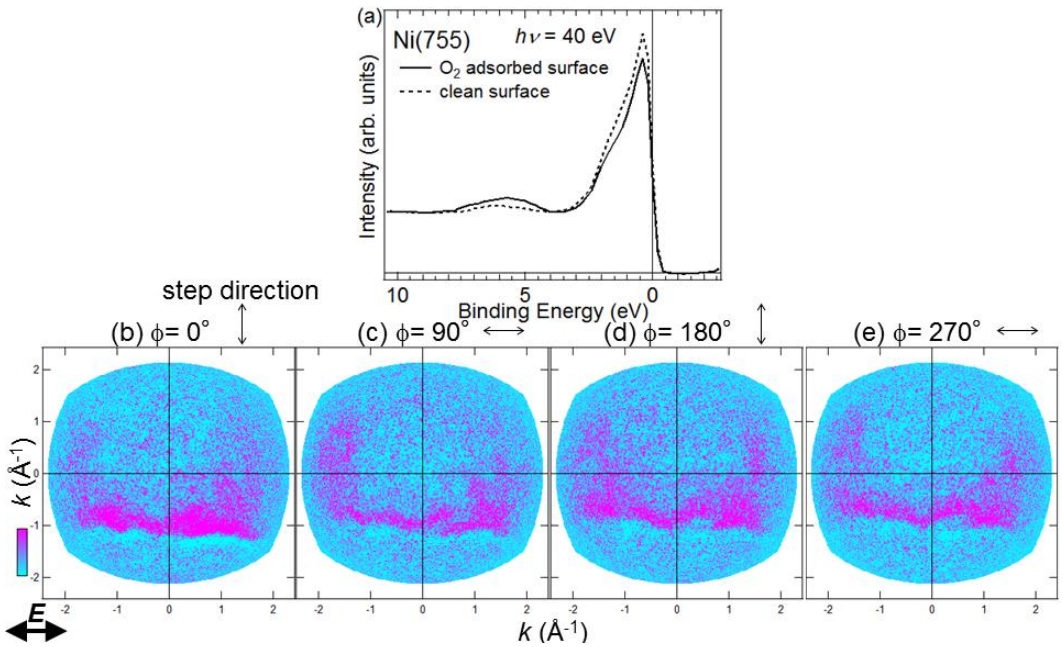

Fig. 1 2D-PES results of Ni(755) stepped surfaces with oxygen adsorption. (a) Angle-integrated PES spectra. The divided PIADs around the binding energy of 6 eV of the sample rotation angles ϕ = 0° (b), 90° (c), 180° (d), and 270° (e). The step directions are also indicated. The electric vector of the incident light is in the horizontal direction.

states hardly changed. Dividing the PIADs around the binding energy of 6 eV for the O_2 adsorbed surface by those for the clean surface [Fig. 1(b)-(e)], we found that the photoelectron intensity around the both side regions are slightly strong independent of the sample rotation angles ϕ. The horizontal line may be due to the experimental apparatus and/or analysis problems judging from the symmetry consideration. This asymmetry of PIAD can be due to the matrix-element effect. Considering the PIADs from atomic orbitals [6], the electronic state of the Ni-O surface complex seems to be composed of *p*-orbital normal to the surface (p_z).

4. Conclusion

We have performed two-dimensional photoelectron spectroscopy measurements on Ni(755) stepped surface with O_2 adsorption. From slightly asymmetric photoelectron intensity angular distributions, we suggest that the electronic state of the Ni-O surface complex is composed of *p*-orbital normal to the surface.

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