Non-dipole Effect and Recoil Effect in High Energy Photoemission

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Based on new synchrotron radiation sources, hard X-ray photoelectron spectroscopy has been employed to study bulk electronic structures. However, high-energy photoemission excited by hard X-ray raises some problems such as breakdown of the electric dipole (E1) approximation and recoil effects. We try to review the previous results on these problems discussed in the two papers[1,2].

1. Non-dipole effect

In this work, the angular distribution of emitted photoelectrons is theoretically studied for high-energy X-rays where electric quadrupole and magnetic dipole transitions are taken into account in addition to the electric dipole transition. For multipole expansion of photon field, power series expansion is commonly used, $\exp(iqx) \approx 1 + iqx + \cdots$. Whereas it is known that this expansion causes mixture of various multipoles. On the contrary irreducible tensor gives proper expansion. We apply irreducible tensor expansion of photon field to estimate accuracy of the power series expansion. Numerical calculations for noble gases demonstrate the importance of nondipole contribution in discussing the angular distribution. We find the power series expansion is good unless electric octupole transition plays some important role.

2. Recoil effect

We also discuss the recoil effects of nuclei associated with photoemission, which give rise to the energy shift and broadening of peak on XPS spectra. We use Debye approximation for phonon modes. Including vibrational excitation, we obtain photoemission formula with the recoil effect and the Franck-Condon effect. In simple models (e.g. powder models), we find there is no interference between these effects. The energy shift is coincident with one caused by the recoil of a free atom in the photoemission processes. The broadenings depend on temperature and crystal structure, in contrast to the energy shift. To compare with experimental results, we also show calculated results in high energy scatterings: Good agreement is found.

[1] R. Suzuki, H. Arai, H. Shinotsuka, T. Fujikawa, e-J. Surf. Sci. Nanotech. **3** (2005) 373-378
[2] T. Fujikawa, R. Suzuki, L. Kövér, J. Elect. Spect. Relat. Phenom. **151** (2006) 170-177