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Valence-Band Satellites in Ni

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Introduction

The photoelectron spectrum of Ni shows, besides the ordinary 3*d*-band emission, an extra feature at ~6 eV below the Fermi energy (E_F). Following an original suggestion by Mott, this 6-eV feature is generally attributed to a many-body effect which leaves two correlated 3*d* holes. So far the 6-eV binding-energy two-hole bound state has been intensively studied and its nature of atomically d^8 multiplet structure was clarified. Although he d^8 multiplet structure has ^1S, ^1G, ^3P, ^1D, and ^3F terms, the 6-eV satellite consists only of ^1G, ^3P, ^1D, and ^3F multiplets. The ^1S state with a binding energy a few eV greater than the 6-eV centroid was not clearly observed in Ni. Its observation is necessary to confirm the Mott's interpretation.

We report an observation of the sharp d^8 ^1S peak and absence of three- and four-hole satellites in Ni [1].

Experiment

The photoemission measurements were carried out at the beamline BL-3B of the Photon Factory. The clean Ni(100) and Ni(111) surfaces, having sharp (1×1) LEED patterns with low backgrounds, were prepared by repeated cycles of Ar^+-ion sputtering and annealing. The amounts of impurities were reduced to less than the detection limit of Auger spectroscopy (e.g., the Auger peak height ratio, O(*KLL*, 510eV)/Ni(*LVV*, 848eV), was less than 1/400 and this corresponds to a coverage of 0.003 monolayer or less).

Results, Discussion and Conclusion

Figure 1 shows a normal-emission spectrum of clean Ni(100) at $h\nu$ =70 eV. A weak but fairly sharp peak is observed at -9.3 eV is assigned to the ^1S term of the d^8 multiplets.

The main 3*d*-line corresponds to the 3*d* hole screened by a 3*d* electron, leading to the final-state configuration of $3d^9 4s$. The satellite corresponds to the two 3*d* holes, which are localized on the same site, screened by 4*s* electrons, leading to the final-state configuration of $3d^8 4s^2$. The 4*s* screening charge reduces the like-charge Coulomb repulsion between the two 3*d* holes and glues the two 3*d* holes together to create a $3d^8$ long-lived bound state. Our data analysis suggests that the Slater-Condon Coulomb integrals are reduced for the d^8 satellite compared to the L_3VV Auger processes and the 6-eV satellite state may mix with the band states.

Three-hole (d^7) and four-hole (d^6) valence-band satellite features have been reported to be observed at ~13.4, ~18, ~22, and ~27 eV below E_F. However, our measurements show that the d^7 and d^6 multiple-hole satellites do not exist or are very weak to be observed. These d^7 and d^6 structures may be extrinsic and perhaps due to artifacts of the subtraction procedures and /or some inelastic electron scattering, *etc*.

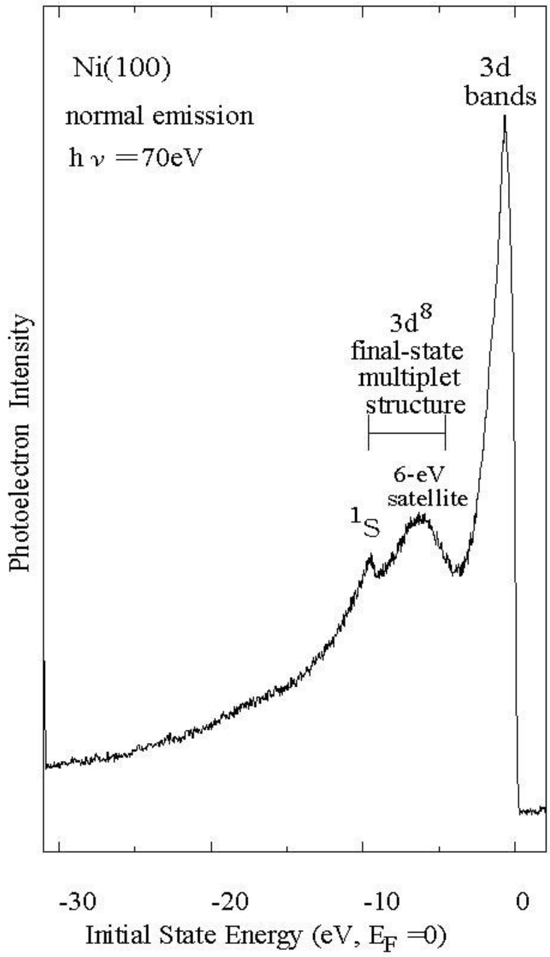

Fig. 1. Normal-emission valence-band spectrum of clean Ni(100) measured at $h\nu$=70 eV.

References

[1] N. Nakajima, S. Hatta, J. Odagiri, H, Kato, and Y. Sakisaka, Phys. Rev. B **70**, 233103 (2004), and references therein.

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