Valence-Band Satellites in Ni

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Introduction
The photoelectron spectrum of Ni shows, besides the ordinary 3d-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 3d 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 the \(d^8\) 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\times1) 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\((KLL, 510eV)/\text{Ni}(LVV, 848eV)\), 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 3d-line corresponds to the 3d hole screened by a 3d electron, leading to the final-state configuration of \(3d^94s\). The satellite corresponds to the two 3d holes, which are localized on the same site, screened by 4s electrons, leading to the final-state configuration of \(3d^84s^2\). The 4s screening charge reduces the like-charge Coulomb repulsion between the two 3d holes and glues the two 3d holes together to create a \(3d^9\) 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.

References

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