Holes in the valence band of copper chalcogenides
Folmer, Jacob Cornelis Willem

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SUMMARY

In its compounds with F, O, Cl and Br copper is known to occur both in the divalent (d⁹) and the monovalent (d¹⁰) state, but with iodine only CuI with monovalent copper is known. Reaction of Cu⁺² and I⁻ in solution yields CuI and I₂ by a redox reaction. The electronegativities of S and Se are comparable with that of iodine; surprisingly enough copper chalcogenides do exist with a composition that – at first view – might indicate the presence of divalent Cu. This thesis deals with these compounds. In Chapter III it is known by XPS that in these compounds the configuration of Cu is essentially d¹⁰; so that one should describe them as compounds of monovalent copper. The compounds do share one peculiar characteristic: the deficit of electrons is present in the form of holes in the valence band which is formed mainly by anion p orbitals.

In the first chapter a general introduction is given to the copper chalcogenides and the phenomenon of "pseudo-divalency". As the study of the valence state of the constituting atoms was mainly performed by means of XPS (X-ray photoelectron spectroscopy), a short introduction to the way this method was applied is given in Chapter II.

The Chapters IV-VI contain more extended studies on the implications of pseudo-divalency and the occurrence of holes in the valence band of copper pyrites, layered copper chalcogenides, and in the spinel CuV₂S₄, respectively. In Chapter V it is also shown that valence-band holes can be polarized by local magnetic moments and – in their turn – can act as a strong parallel coupling medium.