THEORY OF SPIN POLARISED AUGER ELECTRON SPECTROSCOPY OF FERROMAGNETIC 3d–TRANSITION METALS

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Auger spectra of ferromagnetic 3d-transition metals are calculated by treating a multi-band Hubbard model. The hopping and overlap integrals of the Hamiltonian are taken from LDA-calculations. The Coulomb integrals for the valence-valence (VV) interaction among the well localised 3d-electrons are expressed in terms of effective Slater parameters (F^0, F^2, F^4). To take into account the core-hole screening in the initial state and the sudden response of the valence electrons due to the destruction of the core hole in the final state, the Hamiltonian is extended by a core-valence (CV) interaction. The problem is solved by means of perturbation theory in the interaction strength for the indirect as well as for the direct correlation.

As an example the theory is evaluated numerically for Ni. We analyse the temperature dependence of the total line shape, the spin polarisation of the Auger electrons and the angular momentum character of the final-state holes. For the ferromagnetically ordered state as well as for temperatures above T_{C}, the Auger spectrum is found to be strongly affected by VV and CV correlations.

We also discuss the UPS and BIS spectra. The screening of the initial state considerably modifies the local density of states and thereby leads to a significant decrease of the local magnetic moment. Eventually, this implies a diminished polarisation of the Auger electrons.

9.7 cm

13.4 cm

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