

THE COVALENT-BAND DESCRIPTION
OF γ -RESONANCE IN $3d$ -
AND $4f$ -FERROMETALS

A. I. Mitsek

Institute for Metal Physics, Nat. Acad. Sci. of Ukraine
(36, Academician Vernadsky Blvd.,
Kyiv 03142, Ukraine)

S u m m a r y

The hybridization of ns -shells with covalent and band electrons is calculated in the multielectronic operator spinors (MEOS) representation. The density of ns -electrons on a nucleus $\rho(0)$ is dependent on covalent bonds. The hyperfine field (HF) B_{HF} is expressed through the spin polarization of ns -electrons. The Hund exchange of an ion Fe^{57} gives $B_{\text{HF}} \sim S_T$, where S_T is the mean spin. In heavy rare earth metals (REM), the spin-orbital $ns^{-4} f$ -contribution is added. It causes a large B_{HF} and the dependence on temperature T as $B_{\text{HF}}(T) \sim J_T$, where J_T – angular moment of an RE ion. Chemical (covalent) bond fluctuations (CBF), responsible for Fe polymorphism, define a linear dependence on T for the chemical shift of a line of γ -resonance in α -Fe and iron compounds. The large energy gap in CBF spectra stabilizes the hcp lattice of heavy REM. The received results interpret experimental data.