THE XANES K-EDGE SPECTRA FOR HgMnSe AND HgFeSe*

A. Kisiel, J. Oleszkiewicz, J. Goniakowski, R. Markowski

Institute of Physics, Jagellonian Uniwersity, Reymonta 4, 30–059 Kraków, Poland

E. Burattini

Laboratori Nazionali di Frascati INFN, Frascati, Italy

G. Dalba

Dipartimento di Fisica, Universitá di Trento, Povo, Italy

AND F. Rocca

Centro di Fisica degli Stati Aggregati ed Impianto Ionico, Tranto, Italy

X-ray absorption near-edge structure for $Hg_{1-x}Mn_xSe$ and $Hg_{1-x}Fe_xSe$ was studied with the use of synchrotron radiation. The self-consistent, semirelativistic LMTO method within the LD approximation was used to calculate electronic band structure and K-edge spectra of these semimagnetic semiconductors. The theoretical results for X-ray absorption spectra were compared with experimental data.

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XANES measurements have been carried out with the use of synchrotron radiation at the ADONE WIGGLER facility in Frascati [1] utilizing the Si(111) and Si(220) channel-cut crystal monochromators. The original samples were high purity $Hg_{1-x}Mn_xSe$ $(x = 0.2)$ and $Hg_{1-x}Fe_xSe$ $(x = 0.1)$ monocrystals grown by Bridgman method. In order to obtain thin specimens of the controlled thickness and homogeneity as required by X-ray absorption technique the samples were finely powdered and deposited on polyacetate films. XAS measurements have been carried out on Se, Mn, Fe K edges. In the experiment the "thickness effect" was negligible [2]. The samples used had the surface density from about 1.5 to 7.0 mg/cm^2.

The maximum values of $\Delta\mu x$ for Se edge attained 0.12–0.15 and 0.06–0.03 for Mn and Fe K edges, respectively. The energy resolution of the experimental set-up of the type used by us is limited by a finite vertical divergence of the photon beam and the finite width of the rocking curve of the monochromatic crystal. The resulting instrumental Gaussian broadening of the half natural width of all measured edges has been estimated to be from 1.22 eV for Se and about 0.8 eV for Fe and Mn K edges. The contribution of each edge to the absorption coefficient has been isolated by extrapolating the pre-edge region to higher energies by a Victoreen-like and by substracting the fitted curve from the remaining experimental spectrum [3]. Figures 1 and 2 present the results for the Se K and Fe K X-ray absorption
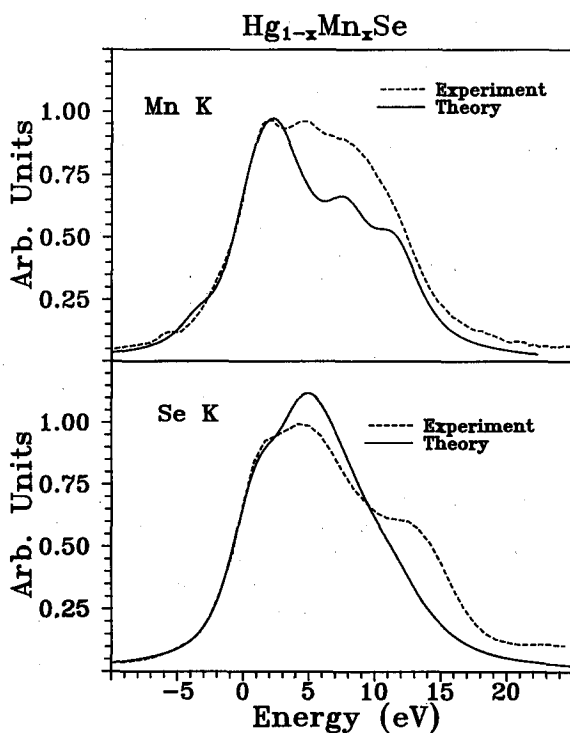

Fig. 1.   Results for the Se K and Fe K of HgFeSe X-ray absorption edges.

edges of HgFeSe and for the Se K and Mn K of HgMnSe, respectively (after substraction of the pre-edge contribution and normalization of the energy scale to the first inflection point at the edge). In order to compare our experimental results with theoretically calculated absorption edges we have applied the procedure of the experimental data reduction reported earlier [4]. This approach provides a direct comparison of the experimental data with results derived from the projected density of states calculated in limited energy range (up to cut-off energy $\epsilon = 17.0$).
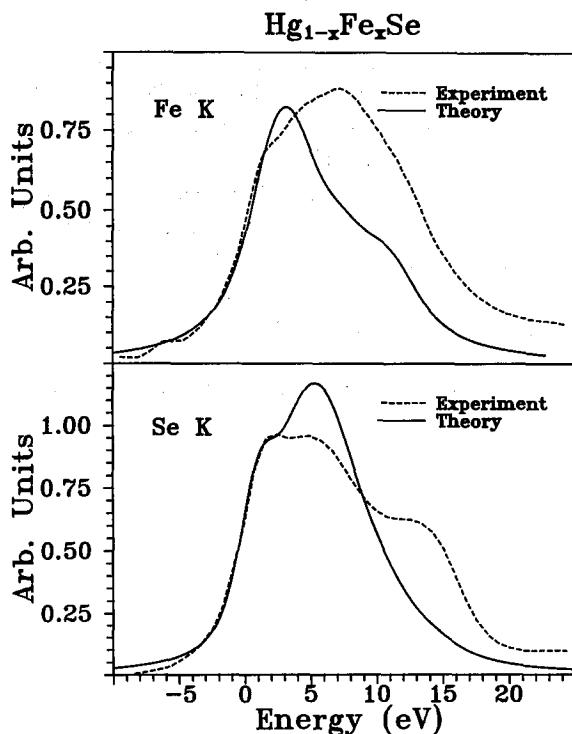
$Hg_{1-x}Fe_xSe$

Fig. 2. Results for the Se K and Mn K of HgMnSe X-ray absorption edges.

The bands and density of states have been obtained using the self-consistent, semirelativistic LMTO method [5, 6]. The exchange-correlation local spin density approximation (LSDA) potential was used in the form proposed by Vosko, Wilk and Nusair [7]. The openness of the zinc-blende structure was dealt in standard way by placing additional "empty spheres" into the unit cell. The calculations were carried out for the antiferromagnetic phase in the hypothetical simple lattice. The results of such band structure calculation formed a basis for X-ray absorption spectra calculation.

The theoretical results describe the experimental data quite satisfactorily except the case of Fe K edge. The main reasons of that discrepancy are limitations of the applied computational method, caused by too small basis function set. The conventional basis function set does not contain the conduction states in higher energy region. In order to adjust the LMTO method for future XANES calculations, the basis function set should be enlarged. Such a modification of the standard LMTO method is generally not trivial. The next reason of existing disagreement is due to the fact that calculations have been performed for different Mn and Fe concentrations than measured in experiment. The differences in concentrations manifest themselves in calculated lattice parameters and this (due to the hybridization) causes changes in the projected density of states.

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