SOFT X-RAY EMISSION SPECTRA OF YA12 AND GdAl2
E. Sobczak, H. Müller

To cite this version:


HAL Id: jpa-00227293
https://hal.science/jpa-00227293
Submitted on 1 Jan 1987

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
SOFT X-RAY EMISSION SPECTRA OF YAl$_2$ AND GdAl$_2$

E. SOBCZAK and H. MÜLLER*

Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, PL-02 668 Warsaw, Poland
*Institute of Experimental Physics, Technical University of Wien, Karlsplatz 13, A-1040 Wien, Austria

The Al L$_{2,3}$ x-ray emission band spectra from YAl$_2$ and GdAl$_2$ have been measured using a soft x-ray grazing incidence grating spectrometer with resolution 0.2 eV. The Al L$_{2,3}$ spectrum of GdAl$_2$ shows a splitting of the band near the valence band top and decreasing of the density of electron states at the Fermi level in comparison to YAl$_2$.

An x-ray band spectrum is produced through electron transitions involving an atomic core state and states lying in the valence band. One of the important uses of the soft x-ray spectroscopy is the extraction from the spectra an information on the electronic band structure of solids, which would otherwise not be available. Such information includes bandwidths, Fermi energies and local partial densities of states. The x-ray data can be used to the verification of band theories.

The intermetallic compounds YAl$_2$ and GdAl$_2$ belong to a large group of rare-earth metal compounds in the cubic Laves phase (i.e., MgCu$_2$ - type structure). The lattice constant $a$ is equal 7.900 and 7.862 Å for GdAl$_2$ and YAl$_2$ respectively (1,2).

The nonmagnetic compound YAl$_2$ was investigated by different methods, but relatively little experimental and theoretical work on electronic structure of YAl$_2$ has been carried out. The Al L$_{2,3}$ x-ray emission from YAl$_2$ was published briefly by Pfleigl et al. (3). Calculations of the electron band structure of YAl$_2$ were reported by Switendick (4) and Hasegawa and Yanase (5).

GdAl$_2$ is ferromagnetic with a transition temperature $T_c = 168 - 171$ K, an effective moment of 7.94 $\mu_B$, and a saturation moment $\mu_{\text{sat}} = 7.2$ $\mu_B$ (1,6,7). The electronic band structure of GdAl$_2$ has not been calculated till present. The x-ray photo-electron spectra of GdAl$_2$ were studied by Kowalczyk (8). The Al K$_{\alpha1,2}$, Al K$\beta$ and Al L$_{2,3}$ x-ray emission spectra from GdAl$_2$ were measured by Wiech and Zöpf (9). The Al L$_{2,3}$ x-ray emission spectrum and x-ray bremsstrahlung isochromat of GdAl$_2$ were reported by Slebarski et al. (10,11).

The aim of this work was to study the Al L$_{2,3}$ x-ray emission band from both YAl$_2$ and GdAl$_2$ intermetallic compounds and to discover the influence of the Gd 4f electrons on the density of electron states in the valence band of GdAl$_2$. The YAl$_2$ was
chosen here as a reference compound for GdAl₂. The yttrium ion has chemical and physical properties similar to gadolinium ion. The main difference is the presence of 4f electrons in the gadolinium ion. One can expect, from the literature, that the difference in the Al L₂,₃ emission band would be not big, therefore measurements have to be performed with high resolution and accuracy.

The Al L₂,₃ emission spectra were measured with a computerized soft x-ray grating spectrometer using primary electron excitation. The radius of the Rowland circle was 1 m; a blazed grating with blazing angle 3°31' and with 600 grooves/mm was used. The incident electron beam and the x-ray beam measured were normal to the sample surface to minimize the x-ray self-absorption and surface contamination effects. The resolution of the spectrometer was about 0.2 eV. The spectra were measured in a step-scanning mode with 0.1 eV/10 sec steps. The power of the x-ray tube was 3 kV, 5 mA. Using turbomolecular pumps the vacuum in the range 10⁻⁵ Pa was obtained. The details of the spectrometer have been described by Goldstein et al. (12,3).

Polycrystalline samples of GdAl₂ and YAl₂ were prepared from Al (99.999%), Gd (99.9%) and Y (99.9%) metals by RF-levitation melting in a water-cooled copper boat under argon atmosphere. The x-ray diffraction analysis did not reveal the presence of any foreign phase. The platelets of thickness about 1.5 mm and diameter about 12 mm were cut and mechanically polished. Each spectrum was recorded through 8 scans. The count rate at maximum was about 4000 counts/80 sec and 2000 counts/ 80 sec for YAI₂ and GdAI₂ respectively.

The Al L₂,₃ x-ray emission band results from electron transitions from the valence band to the Al L₂,₃ core hole. Due to the dipole selection rules the s and d electron state density around an aluminum atom can be studied by the Al L₂,₃ emission band.

In Fig. 1 the Al L₂,₃ emission band spectrum from GdAl₂ is shown. The intensity is evaluated as countrate/\nu².

In Fig. 2 the Al L₂,₃ emission band spectrum from YAI₂ is shown. One of the peaks is the Y M₅ line (132.47 eV) reflected in second order of diffraction. Our spectrum from YAI₂ seems to be measured with better resolution than the spectrum published by Pfliegl et al. (3). In order to substract the Y M₅ line from the Al L₂,₃ spectrum, the Y M₅ spectrum from Y-metal has been measured (the lower curve in Fig. 2). The subraction was performed by computer fitting method. The Y M₅ line from Y-metal is shifted by 0.03 eV relatively to that one from YAI₂.

After the Y M₅ subraction, the background correction and normalization to the main maximum have been performed for the spectra from GdAl₂ and YAI₂ samples (Fig. 3). Characteristic parameters of the fine structure of the Al L₂,₃ emission bands from both intermetallic compounds are presented in Table 1. Our parameters agree well
with those of Wiech and Zöpf (9). However their parameters are inconsistent with the spectrum shown in Fig. 7 in their paper. We were informed by Professor Wiech, that a mistake occurred in the caption of the Fig. 7.

Fig. 3. The experimental Al L\textsubscript{2,3} emission bands from GdAl\textsubscript{2} and YAl\textsubscript{2} after corrections and theoretical Al L\textsubscript{2,3} spectrum of YAl\textsubscript{2} calculated by K.-H. Schwarz and P. Mohn (unpublished).

Fig. 4. Comparison of the Al L\textsubscript{2,3} emission spectra from YAl\textsubscript{2} and GdAl\textsubscript{2} in the vicinity of the Fermi level.

TABLE 1.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Fermi energy (eV)</th>
<th>Position of maxima</th>
<th>Relative intensity</th>
<th>Band width (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>A</td>
<td>B</td>
<td>C</td>
</tr>
<tr>
<td>YAl\textsubscript{2}</td>
<td>72.4</td>
<td>65.0</td>
<td>68.4</td>
<td>71.6</td>
</tr>
<tr>
<td>GdAl\textsubscript{2}</td>
<td>72.4</td>
<td>65.3</td>
<td>68.4</td>
<td>71.5</td>
</tr>
<tr>
<td>GdAl\textsubscript{2} (9)</td>
<td>-</td>
<td>65.25</td>
<td>68.40</td>
<td>71.50</td>
</tr>
</tbody>
</table>

Schwarz and Mohn have calculated soft x-ray band spectra of YAl\textsubscript{2} from the electron band structure of YAl\textsubscript{2} (unpublished). Their theoretical Al L\textsubscript{2,3} emission spectrum of YAl\textsubscript{2} is shown in Fig. 3. The main contribution to the intensity of this spectrum is from s-type electron states in the valence band. The d-type electron states contribute to this spectrum mostly in the vicinity of the top of valence band.

When comparing spectra from YAl\textsubscript{2} and GdAl\textsubscript{2} one can see, that the band width is slightly narrower in the case of GdAl\textsubscript{2}, what is connected among others with the bigger lattice constant of GdAl\textsubscript{2}. The intensity ratio of maxima A and B is the same in both compounds, but the maximum A in the GdAl\textsubscript{2} spectrum is shifted by 0.3 eV to higher photon energy, what can be interpreted as a result of interaction of valence
electrons with Gd 4f electrons, which are placed just at energy of 8 eV below the Fermi level (8).

The intensity of maximum C is by 15% smaller in the GdAl₂ spectrum and split of about 0.5 eV in comparison to that of YAl₂ (Fig. 4). The 0.5 eV splitting we interpret not only as the spin-orbital splitting of the Al L₂,₃ core level, but also as a band splitting in the top of valence band, because the intensity ratio of C' and C peaks is much bigger than 1:2. A similar band splitting of about 1 eV was observed near the top of valence band in the x-ray photoelectron spectrum from GdAl₂ by Kowalczyk (8).

The Fermi level is assumed to be at 50% intensity of the first step rise on the high energy side of the Al L₂,₃ emission band. The Fermi energy is equal in both compounds, what means that Al ions are in a very similar potential in both compounds and there is no additional charge shift between Al and Gd ions in GdAl₂ in comparison to YAl₂.

The density of electron states at the Fermi level is about 20% smaller in GdAl₂ than in YAl₂, what we interpret as due to exchange interaction between Gd 4f electrons and p, d valence electrons. The decreasing of the density of electron states near the top of valence band in GdAl₂ without changes of the Fermi energy, we interpret as an electron shift from the d valence band to 4f band, what is consistent with high magnetic moment in GdAl₂.

References