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SOFT X-RAY EMISSION SPECTRA OF YAl₂ AND GdAl₂

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The Al L₂,₃ x-ray emission band spectra from YAl₂ and GdAl₂ have been measured using a soft x-ray grazing incidence grating spectrometer with resolution 0.2 eV. The Al L₂,₃ spectrum of GdAl₂ 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 YAl₂.

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 YAl₂ and GdAl₂ belong to a large group of rare-earth metal compounds in the cubic Laves phase (i.e., MgCu₂ - type structure). The lattice constant a is equal 7.900 and 7.862 Å for GdAl₂ and YAl₂ respectively (1,2).

The nonmagnetic compound YAl₂ was investigated by different methods, but relatively little experimental and theoretical work on electronic structure of YAl₂ has been carried out. The Al L₂,₃ x-ray emission from YAl₂ was published briefly by Pfiegl et al. (3). Calculations of the electron band structure of YAl₂ were reported by Switendick (4) and Hasegawa and Yanase (5).

GdAl₂ is ferromagnetic with a transition temperature Tᵣ = 168 - 171 K, an effective moment of 7.94 μₜ, and a saturation moment μₚsat = 7.2 μₜ (1,6,7). The electronic band structure of GdAl₂ has not been calculated till present. The x-ray photo-electron spectra of GdAl₂ were studied by Kowalczyk (8). The Al K₃,₂, Al Kβ and Al L₂,₃ x-ray emission spectra from GdAl₂ were measured by Wiech and Zöpf (9). The Al L₂,₃ x-ray emission spectrum and x-ray bremsstrahlung isochromat of GdAl₂ were reported by Slebarski et al. (10,11).

The aim of this work was to study the Al L₂,₃ x-ray emission band from both YAl₂ and GdAl₂ intermetallic compounds and to discover the influence of the Gd 4f electrons on the density of electron states in the valence band of GdAl₂. The YAl₂ was...
chosen here as a reference compound for GdAl$_2$. 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 L$_{2,3}$ emission band would be not big, therefore measurements have to be performed with high resolution and accuracy.

The Al L$_{2,3}$ 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 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 GdAl$_2$ and YAl$_2$ 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 YAl$_2$ and GdAl$_2$ respectively.

The Al L$_{2,3}$ x-ray emission band results from electron transitions from the valence band to the Al L$_{2,3}$ 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 L$_{2,3}$ emission band.

In Fig. 1 the Al L$_{2,3}$ emission band spectrum from GdAl$_2$ is shown. The intensity is evaluated as countrate/$\nu^2$.

In Fig. 2 the Al L$_{2,3}$ emission band spectrum from YAl$_2$ is shown. One of the peaks is the Y M$_{5}$ line (132.47 eV) reflected in second order of diffraction. Our spectrum from YAl$_2$ seems to be measured with better resolution than the spectrum published by Pfliegl et al. (3). In order to substract the Y M$_{5}$ line from the Al L$_{2,3}$ spectrum, the Y M$_{5}$ spectrum from Y-metal has been measured (the lower curve in Fig. 2). The substraction was performed by computer fitting method. The Y M$_{5}$ line from Y-metal is shifted by 0.03 eV relatively to that one from YAl$_2$.

After the Y M$_{5}$ subtractions, the background correction and normalization to the main maximum have been performed for the spectra from GdAl$_2$ and YAl$_2$ samples (Fig. 3). Characteristic parameters of the fine structure of the Al L$_{2,3}$ 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.

![Graph showing Al L2,3 emission bands from GdAl2 and YAl2 after corrections and theoretical Al L2,3 spectrum of YAl2 calculated by K.-H. Schwarz and P. Mohn (unpublished).](image1)

![Graph showing comparison of the Al L2,3 emission spectra from YAl2 and GdAl2 in the vicinity of the Fermi level.](image2)

**Fig. 3.** The experimental Al L2,3 emission bands from GdAl2 and YAl2 after corrections and theoretical Al L2,3 spectrum of YAl2 calculated by K.-H. Schwarz and P. Mohn (unpublished).

**Fig. 4.** Comparison of the Al L2,3 emission spectra from YAl2 and GdAl2 in the vicinity of the Fermi level.

**Table 1.** Characteristic parameters of the fine structure of the Al L2,3 emission spectra from YAl2 and GdAl2 (in eV).

<table>
<thead>
<tr>
<th>Sample</th>
<th>Fermi energy</th>
<th>Position of maxima</th>
<th>Relative intensity</th>
<th>Band width</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(eV)</td>
<td>A</td>
<td>B</td>
<td>C</td>
</tr>
<tr>
<td>YAl2</td>
<td>72.4</td>
<td>65.0</td>
<td>68.4</td>
<td>71.6</td>
</tr>
<tr>
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<td>65.3</td>
<td>68.4</td>
<td>71.5</td>
</tr>
<tr>
<td>GdAl2 (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 YAl2 from the electron band structure of YAl2 (unpublished). Their theoretical Al L2,3 emission spectrum of YAl2 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 YAl2 and GdAl2 one can see, that the band width is slightly narrower in the case of GdAl2, what is connected among others with the bigger lattice constant of GdAl2. The intensity ratio of maxima A and B is the same in both compounds, but the maximum A in the GdAl2 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