GIANT HYPERFINE FIELD AT THE ANTIMONY SITE IN THE HEUSLER-ALLOY Pd₂MnSb

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Received 28 January 1972

The magnetic hyperfine field at ¹²¹Sb in Pd₂MnSb has the anomalously large value (at 100 K) of ±579 ±5 kG. In the closely related compound PdMnSb we find ±302 ±5 kG, similar to other ferromagnetic intermetallics containing Mn and Sb.

The ferromagnetic (Tc = 247 K) Heusler compound Pd₂MnSb has the L₂₁ structure, with a magnetic moment of 4.4 μB per formula unit, confined to the Mn atom [1-3]. We find that the ¹²¹Sb hyperfine field in Pd₂MnSb is much larger in magnitude than any Sb hyperfine field reported to date. This giant hyperfine field is much larger than expected on the basis of previous measurements of Sb and Sn hyperfine fields in Heusler and other alloys. The Sb hyperfine field in the closely related alloy PdMnSb (ferromagnetic, Tc = 500 K, C₁₅ structure [4]) is found to be within the normal range of experience.

Hyperfine fields and isomer shifts were measured at 100 K using the ¹²¹Sb Mössbauer effect. The spectrometer was calibrated using the hyperfine field value [5, 6] of +291 kG for Sb in NiMnSb at 100 K. Isomer shifts were measured with respect to an InSb absorber at 100 K. The compounds were prepared by arc melting in a Ti-gettered argon atmosphere, followed by a 48 hr anneal at 1070 K and slow cooling. Metallo-

<table>
<thead>
<tr>
<th>Compound</th>
<th>a₀</th>
<th>Tc</th>
<th>Hn</th>
<th>Γ</th>
<th>Isomer shift</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(nm)</td>
<td>(K)</td>
<td>(kG)</td>
<td>(mm/sec)</td>
<td>(mm/sec)</td>
</tr>
<tr>
<td>Pd₂MnSb</td>
<td>0.6419</td>
<td>247 [2]</td>
<td>±579</td>
<td>4.8</td>
<td>1.1</td>
</tr>
<tr>
<td>PdMnSb</td>
<td>0.6235</td>
<td>500 [4]</td>
<td>±302</td>
<td>3.5</td>
<td>0.7</td>
</tr>
<tr>
<td>NiMnSb</td>
<td>0.5913</td>
<td>720 [11]</td>
<td>+291 [5]</td>
<td>3.1</td>
<td>1.4</td>
</tr>
</tbody>
</table>
the Sb field is nearly the same for an Sb on a Pd site as for an Sb on an Sb site. A similar behavior has been reported [8] for the Ni hyperfine field in Ni2MnSn, where the Ni field is relatively unchanged by Ni-Sn disorder. The excess linewidth for Pd2MnSb (table 1) could be attributed to the disorder and allows a distribution in hyperfine fields of approximately ±20 kG centered around the nominal value of 579 kG.

The great difference in the Sb magnetic hyperfine field between Pd2MnSb and PdMnSb is in contrast to previous results [5] for the isoelectronic L21 and C1b structures Ni2MnSb and NiMnSb, which both have nearly the same magnitude (and the same positive sign, ~+300 kG) for the Sb field. It is further interesting to note that the field of Sn in Pd2MnSn (±48 kG[9]) is lower in magnitude than that of Sn in Ni2MnSn (±93 kG[10]), whereas the field found here for Sb in Pd2MnSb (±579 kG) is much higher in magnitude than that for Sb in Ni2MnSb (+302 kG[5]). Since most of the signs have not yet been determined, the direction of these changes in field values cannot be compared.

In table 2 derived antimony site hyperfine field coupling constants for a number of intermetallic compounds are compared. An explanation of the enhanced coupling in Pd2MnSb based on differences in the local charge density at Sb does not appear tenable since the 121Sb isomer shift in Pd2MnSb is well within the range of values observed for other Sb Heusler alloys.

Table 2

<table>
<thead>
<tr>
<th>Compound Structure</th>
<th>Ferromagnetic saturation moment, (µB) (per formula unit)</th>
<th>Derived hyperfine field coupling constant (kG/µB) (per formula unit)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pd2MnSb L21</td>
<td>4.4 [2]</td>
<td>138</td>
</tr>
<tr>
<td>Ni2MnSb L21</td>
<td>3.6 [12]</td>
<td>86</td>
</tr>
<tr>
<td>PdMnSb C1b</td>
<td>4.0 [13]</td>
<td>77</td>
</tr>
<tr>
<td>NiMnSb C1b</td>
<td>3.8 [12]</td>
<td>78</td>
</tr>
<tr>
<td>MnSb B81</td>
<td>3.3 [14]</td>
<td>107</td>
</tr>
</tbody>
</table>

A possible explanation might be that the Pd atoms in Pd2MnSb attain a small moment. This small Pd moment might serve to enhance the hyperfine field transfer to the Sb atoms. However, in Co2MnSn, where the Co is known to carry a magnetic moment, there is no such enhancement. The Sn hyperfine field is +107 kG[15], which is only slightly greater than the 93 kG[10] for Sn in Ni2MnSn. A firm explanation for the giant hyperfine field in Pd2MnSb is not readily apparent (but might be related to the unusual pressure dependence of TC[16]).

The authors thank Dr. R. E. Watson and Dr. L. H. Bennett for useful comments.

References