GIANT HYPERFINE FIELD AT THE ANTIMONY SITE IN THE HEUSLER-ALLOY Pd_2MnSb

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The magnetic hyperfine field at ^{121}Sb in Pd_2MnSb 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 (T_c = 247 K) Heusler compound Pd_2MnSb has the $L2_1$ structure, with a magnetic moment of 4.4 μ_B per formula unit, confined to the Mn atom [1-3]. We find that the ^{121}Sb hyperfine field in Pd_2MnSb 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, T_c = 500 K, $C1_b$ structure [4]) is found to be within the normal range of experience.

Hyperfine fields and isomer shifts were measured at 100 K using the ^{121}Sb 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. Metallographic analysis showed each sample to be predominantly single phase, with less than about 5% of an undetermined second phase detected at grain boundaries. X-ray analysis showed that both alloys were cubic, with the appropriate superlattice lines expected for the $L2_1$ (Heusler) and $C1_b$ structures. The measured lattice constants (table 1) are in good agreement with previously reported values [1,4].

The Mössbauer spectra of Pd_2MnSb, PdMnSb and NiMnSb are shown in fig. 1. The solid lines are least squares fits to the spectra assuming a single value of magnetic hyperfine field. The measured hyperfine fields, linewidths and isomer shifts are given in table 1. The value of H_n for Pd_2MnSb, extrapolated to 0 K by using the magnetization curve [2], is 609 kG, much larger than the highest Sb magnetic hyperfine field found to date [7] of 352.5 kG in MnSb.

The considerable Pd-Sb disorder reported [2] for Pd_2MnSb is consistent with the single valued hyperfine field found here if it is postulated that

Table 1
Comparison of Pd_2MnSb, PdMnSb and NiMnSb. Mössbauer effect data were obtained at 100 K. Isomer shifts are given with respect to an InSb absorber at 100 K. Lattice constants, a_o', were measured at 300 K.

Compound	a_o (nm)	T_c (K)	H_n (kG)	Γ (mm/sec)	Isomer shift (mm/sec)
	(±0.001)		(±5)	(±0.2)	(±0.2)
Pd_2MnSb	0.6419	247 [2]	±579	4.8	1.1
PdMnSb	0.6235	500 [4]	±302	3.5	0.7
NiMnSb	0.5913	720 [11]	+291 [5]	3.1	1.4

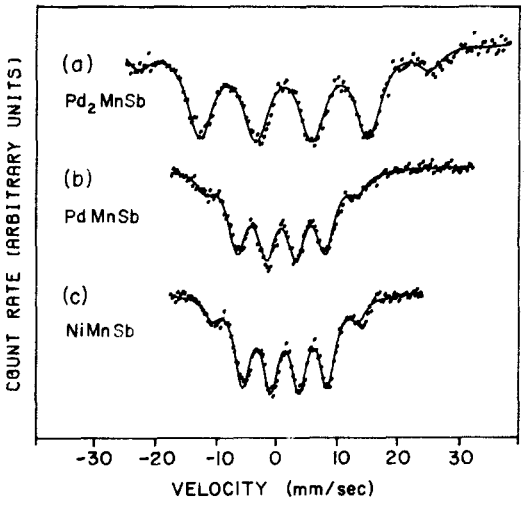

Fig. 1. ^{121}Sb Mössbauer effect absorption spectra at 100 K. In each case the solid line represents a least squares fit to a single magnetic hyperfine field. The zero of velocity represents the center of an InSb absorber at 100 K.

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 Ni_2MsSn, where the Ni field is relatively unchanged by Ni-Sn disorder. The excess linewidth for Pd_2MnSb (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 Pd_2MnSb and PdMnSb is in contrast to previous results [5] for the isoelectronic $L2_1$ and $C1_b$ structures Ni_2MnSb 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 Pd_2MnSn (±48 kG[9]) is lower in magnitude than that of Sn in Ni_2MnSn (±93 kG[10]), whereas the field found here for Sb in Pd_2MnSb (±579 kG) is much higher in magnitude than that for Sb in Ni_2MnSb (+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 Pd_2MnSb based on differences in the local charge density at Sb does not appear tenable since the ^{121}Sb isomer shift in Pd_2MnSb is well within the range of values observed for other Sb Heusler alloys.

Table 2
Comparison of the antimony site hyperfine field coupling constants in Heusler-type alloys and in MnSb, derived from the saturation moments and 0 K Sb hyperfine field.

Compound	Structure	Ferromagnetic saturation moment, (μ_B) (per formula unit)	Derived hyperfine field coupling constant (kG/μ_B) (per formula unit)
Pd_2MnSb	$L2_1$	4.4 [2]	138
Ni_2MnSb	$L2_1$	3.6 [12]	86
PdMnSb	$C1_b$	4.0 [13]	77
NiMnSb	$C1_b$	3.8 [12]	78
MnSb	$B8_1$	3.3 [14]	107

A possible explanation might be that the Pd atoms in Pd_2MnSb attain a small moment. This small Pd moment might serve to enhance the hyperfine field transfer to the Sb atoms. However, in Co_2MnSn, 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 Ni_2MnSn. A firm explanation for the giant hyperfine field in Pd_2MnSb is not readily apparent (but might be related to the unusual pressure dependence of T_c [16]).

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