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129 I TRANSFERRED MAGNETIC HYPERFINE FIELD IN THE $\beta$-IRON TELLURIDE ($Fe_{1+x}Te$)

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INTRODUCTION - There is considerable interest in transition metal tellurides which order magnetically. In principal such systems can be studied by means of $^{125}$Te Mössbauer spectroscopy, but this has not proved particularly successful because of the large natural linewidth associated with the transition /1,2/. An alternative approach, is to make use of the $^{129}$I Mössbauer transition which has a much narrower natural linewidth and hence superior resolution. In tellurium compounds this is achieved by preparing the compound of interest with $^{128}$Te, carrying out a neutron irradiation to produce $^{129}$Te or $^{129}$mTe which populates the $^{129}$I Mössbauer excited state, and using this material as a source to carry out the experiment /3/. We have used this method to study the hyperfine field transferred to the iodine atom, on a tellurium site, in $\beta$-Iron telluride ($Fe_{1+x}Te$).

Experimental - High purity iron powder was first reduced under hydrogen in an alumina boat, then mixed with tellurium powder (either natural Te or enriched to $>99\%$ in $^{128}$Te obtained from Oak Ridge) in an atomic ratio Te/Fe = 0.8. The finely powdered mixture was pressed into a pellet, placed in a closed alumina crucible and sealed in a silica tube under vacuum ($10^{-6}$torr). Samples were heated in a furnace at a rate of 50°/hr to 600°C, annealed at 600°C for 12 hrs, cooled at a rate of 100°/hr to 300°C and annealed for 40 hrs. The sample was finally cooled at 25°/hr to room temperature. During the thermal processing the sample remained in the coolest part of the evacuated silica tube so that the sample temperature could not exceed 600°C. The sample was powdered and a small amount of unreacted iron was removed magnetically. The x-ray diffraction powder pattern (CuK$_\alpha$ radiation) of the non-enriched control sample only exhibited lines belonging to the $\beta$-iron telluride /4/. $^{57}$Fe Mössbauer spectra were measured for the non-enriched sample at 295 K, 80 K and 6 K versus a $^{57}$Co(Rh) source. The spectra obtained are in substantial agreement with the previous data though our room temperature spectrum is much less asymmetric than the earlier spectrum /5/. The $\delta Fe_{1+x}^{128}$Te gave identical spectra, with IS = 0.32 mm$s^{-1}$; QS = -0.32 mm$s^{-1}$; $\Gamma_l=0.23$ mm$s^{-1}$; and $g_{11}=0.95$ representing the degree of anisotropy in the Debye Waller factor and/or any texture in the sample /6/. Figure 1 shows the 295°K spectrum with a 2.2% Fe$^{2+}$ impurity (IS=1.19 mm$s^{-1}$;
QS=2.49 mms⁻¹) which must arise from reaction with the crucible walls. The 4.2 K spectrum was similar to that of Hermon et al. [5] with a distribution of magnetic fields due to the presence of the interstitial iron: it was not computer fitted.

The sample enriched in ¹²⁸Te (30mg ¹²⁸Te) was then placed in the McMaster reactor for 2 hrs. in a thermal neutron flux of ~10¹³ n.cm⁻²s⁻¹. Spectra were recorded at 80 K and 4.2 K with the irradiated β-iron telluride as a source against a Cu¹²⁹I absorber at the same temperature, and fitted as described in [6]. The spectra are shown in Figure 2. Owing to the close geometry, baseline effects are strong and have been included in the spectral fitting.

From the linewidth and quadrupole coupling constant obtained at 80°K results in IS=1.03 ± 0.05 mms⁻¹; a transferred hyperfine field of 142 K0e with a distribution (δΗ) of 60% ± 7; and <δ> = 64° ± 5. The field distribution is related to the disorder of the iron in the interstitial sites.

The dominant contributions to the field at the iodine are covalent spin density transfer fₛ and fₛ from the closest iron atoms to the iodine 5s and 5p orbitals respectively. The e.f.g. tensor for an iodine atom located at a tellurium site is axially symmetric and its principal component is parallel to the crystal C axis. Leciejewicz [7] has found that the iron magnetic moments are coupled ferromagnetically within the tetragonal planes. Therefore the isotropic field Hₛ must be perpendicular to the C axis, and it is likely that the anisotropic field Hₚₒ is parallel to the C axis. Adopting Pₒ = 150 x 10²⁴ cm⁻³, <r⁻³>=121.5 x 10²⁴ cm⁻³, and Hₚₒ = fₚₒ x 450 (K0e) / 3, we calculate fₛ = 1.1% and fₚₒ = 13.8% for s and pₒ covalent transfer respectively along the Fe-I bond.

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References-