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CDW's AND SDW's IN $\text{Ta}_{0.95}\text{Fe}_{0.05}\text{S}_3$ WITH MAGNETIC FIELDS AT $T = 4.2$ K

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Abstract. – Quasi-one-dimensional $\text{Ta}_{0.95}\text{Fe}_{0.05}\text{S}_3$ has been studied in magnetic fields applied at $T = 4.2$ K by Mössbauer spectroscopy. The amplitudes of the CDW's are increased. Also a phase transition is induced; SDW's then coexist with CDW's.

When an external magnetic field is applied to charge-density-wave (CDW) conductors at low temperature new phenomena are sometimes observed. For example, Parilla *et al.* [1] find an anomalous magneto-resistance in monoclinic NbSe_3 ; it seems the ratio of condensed (CDW's) to normal electrons is increased. When a field of 3.5 kOe is applied to the two-dimensional material 2H-TaS at $T = 1.5$ K evidence for the coexistence of a spin-density wave (SDW) with a CDW was obtained [2].

A Mössbauer study of CDW's in the quasi-one-dimensional family $\text{Ta}_{1-x}\text{Fe}_x\text{S}_3$ has been reported [3]. We now present a study of $\text{Ta}_{0.95}\text{Fe}_{0.05}\text{S}_3$ when an external magnetic field is applied at $T = 4.2$ K.

The sample was made by employing high temperature and high pressure [3]. The crystal structure is monoclinic, the same as for monoclinic TaS_3 and similar to that for NbSe_3 . Six sulfur ions form the corners of a trigonal prism with a Ta ion at the center. Neighboring prisms share triangular faces and are stacked along the *b* axis to form lengthy chains. Three types of prism, designated I, II and III, have different S-S bond lengths in the basal plane perpendicular to the *b* axis, namely 0.2068, 0.2105 and 0.2835 nm, respectively [4]. For the similar compound NbSe_3 , NMR measurements show that chains I and II are in the CDW state and chain III is an insulator [5]. Our earlier Mössbauer data show that the probability of an iron atom in chains I, II and III is 3 : 3 : 4, respectively [3].

The absorber was in the form of a disk of randomly oriented particles immobilized in benzophenone. The external magnetic field was perpendicular to the plane of the disk. The Mössbauer source was Co in a Rh host, a triangular drive was used and the data folded. Since the S-S bonds of chains I and II are nearly equal, the assumption was made that these two chains are in the same CDW state. Also, the iron atoms were assumed to have the same probability to lie in the electron excess region (the peak of the CDW's or P-branch) and the deficient region (the valley of the CDW's, or V-branch) of chains I and II. The number of iron atoms on chain III was fixed at 40 %. It was then found that three patterns provided an adequate fit to each Mössbauer spectrum.

Fig. 1. – Mössbauer spectra (dots) at $T = 4.2$ K in various external magnetic fields. For $H = 0$ and 0.5 kOe 3 doublets are fitted, for higher fields 3 sextets (solid lines).

The Mössbauer spectra obtained as a function of the external magnetic field are shown in figure 1. Clearly, a marked change in the spectra occurs at $H = 10$ kOe, that is, at a threshold field somewhat less than 10 kOe a phase change occurs.

Three doublets are fitted to the spectra at $H = 0$ and 0.5 kOe. For $H \geq 10$ kOe some and perhaps all of the subpatterns are hyperfine-field split. However, because the magnetic and quadrupole interactions are comparable in magnitude and because each spectrum is rather featureless, an unambiguous fitting is difficult. A fit with two sextets and one doublet was

not obtained. A satisfactory fit was provided by three sextets; some simplifying assumptions were needed. The assignments of two subpatterns to the P-branch and V-branch of the I and II chains and the third to chain III are indicated by the bar diagrams in figure 1. It is unexpected that chain III has a hyperfine field; its origin is presumably the interactions with chains I and II.

The hyperfine parameters deduced from the data, viz, the isomer shifts, δ , the quadrupole shifts, ε , and the hyperfine fields, H_{hf} , are plotted in figure 2. The isomer shift of the P-branch decreases and that of the V-branch increases as the external field increases; a small discontinuity occurs at the phase transition. Since the charge density at the Fe nuclei is inversely proportional to δ , it follows that the amplitude of the CDW's increases with H . The implication is that the electronic states near the Fermi level are altered so that the ratio of condensed (CDW) to normal electrons is increased. The isomer shift for chain III is almost unchanged. The quadrupole splitting does increase with H for all patterns; it seems that the lattice distortion increases as the field is increased. The increase for chain III may occur *via* the long-range Coulomb forces with chains I and II.

When a hyperfine field is present it usually follows that magnetic ordering has occurred. The magnetization when $H = 30$ kOe as a function of temperature is shown in figure 3; the data suggest the ordering is antiferromagnetic. Hence, SDW's appear to be induced and coexist with the CDW's.

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Fig. 2. - Hyperfine parameters as a function of external magnetic field applied.

Fig. 3. - The magnetization as a function of temperature. ►