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MAGNETIC SUSCEPTIBILITY AND ^{57}Fe MÖSSBAUER SPECTRA OF $T_{1+x}Nb_{3-x}Se_{10}$ WITH T = Fe, Cr

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Abstract The metal-insulator transition of $Fe_{1+x}Nb_{3-x}Se_{10}$, $0.25 \leqslant x \leqslant 0.40$, and of $Cr_{1.45}Nb_{2.55}Se_{10}$, was studied by measurements of resistivity and magnetic susceptibility. The ^{57}Fe Mössbauer spectra were analysed by the assumption of a statistical distribution of Fe in the octahedral chains.

INTRODUCTION

The resistivity of $Fe_{1+x}Nb_{3-x}Se_{10}$ increases by 9 orders between 140 and 3K[1,2,3]. This increase is supposed to originate from the atomic disorder due to Anderson localization[2]. X-ray diffraction showed the symmetry to be monoclinic and the structure to contain two trigonal prismatic as well as two octahedral chains[2,3,4](FIG. 1). X-ray scattering showed the CDW to be incommensurate with q (0.0, 0.27, 0.0) and the CDW vector is only slightly different from the high temperature CDW in $NbSe_3$. Recently, the first measurements of the physical properties[1,2,3,5] and of the Mössbauer spectra[5] have been reported. Our crystals were prepared by a sublimation method[6].

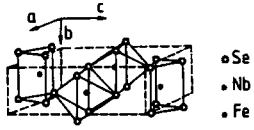

FIG.1 Structure of $FeNb_3Se_{10}$

RESULTS

Whereas $Cr_2Nb_2Se_{10}$ as well as $Fe_{1+x}Nb_{3-x}Se_{10}$ exhibit a resistivity variation of more than 7 orders[2,3,6,7], the resistivity variation of the compound with less Cr-content is remarkably smaller (FIG. 2). The values of the magnetic susceptibility increase with increasing Fe-content of the compound (FIG. 3). At low temperature a Curie contribution to χ appears and can be fitted for $T < 100$ K with the Curie - Weiss expression $\chi = C_g/(T+\theta) + \chi_o$, C_g = Curie-constant, θ = Weisstemperature, χ_o = temperature independent term. $Ti_{0.67}Cr_{1.33}Nb_2Se_{10}$ and $Cr_{1.45}Nb_{2.55}Se_{10}$ powder samples exhibit a high paramagnetic susceptibility behaviour between 77 and 550 K, but no minimum (FIG. 4). $Cr_{1.33}Nb_{2.67}Se_{10}$ below 200 K shows a nearly temperature independent magnetic susceptibility in a magnetic field of 12.1 kOe (FIG. 4).

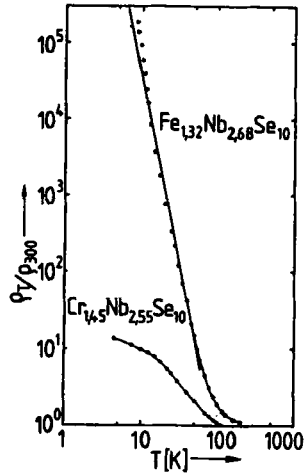

FIG. 2 Resistivity ratio versus temperature

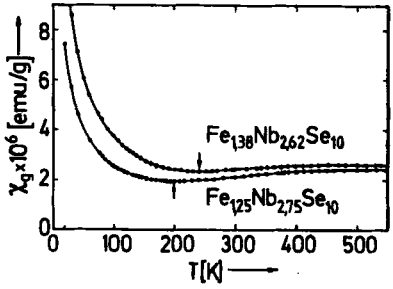

FIG. 3 Magnetic susceptibility versus temperature

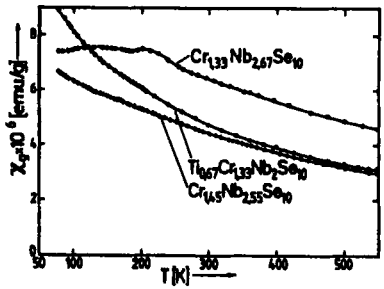

FIG. 4 Magnetic susceptibility versus temperature

For the Mössbaueranalysis the following assumptions were made: i) statistical substitution of Fe only in the octahedral chains, ii) center shift (Is) decreases with increasing temperature due to the influence of second order Doppler shift, iii) quadrupole splitting (Q) mainly determined by the arrangement and number of surrounding Fe atoms.

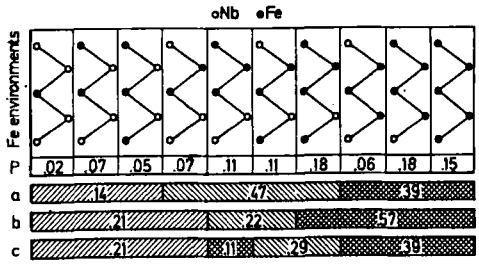

FIG. 5 Fe-environments in the octahedral chains and their abundances (P) for $Fe_{1.25}Nb_{2.75}Se_{10}$ (a) intensity ratio for nearest neighbours; (b),(c) intensity ratios for the selected combinations of nearest and next-nearest environments

Taking into account only nearest neighbours, no fit with the respective intensity ratio of the three subspectra (FIG. 5a) was possible. A fit with nearest and next nearest neighbours leads to ten different environments (FIG. 5). Due to the poor resolution a restriction to only three different subspectra was necessary. Two combinations of the different environments (FIG. 5b,c) lead to the observed intensity ratio fulfilling all other assumptions. For both holds that the smallest value of Q is obtained, if Fe is completely surrounded by Fe. The assumption of statistical substitution of Fe in the octahedral chains is valid for all temperatures and all x for $Fe_{1+x}Nb_{3-x}Se_{10}$. The fit for $Fe_{1.33}Ta_{0.67}Nb_2Se_{10}$ (FIG. 6) indicates that the assumption of Fe(Ta) only in the octahedral chains is not valid for this compound. At 140 K, where the CDW in $Fe_{1.25}Nb_{2.75}Se_{10}$ forms, the obtained values of both Q and Is are not in agreement with those obtained for the other temperatures (FIG. 7). For

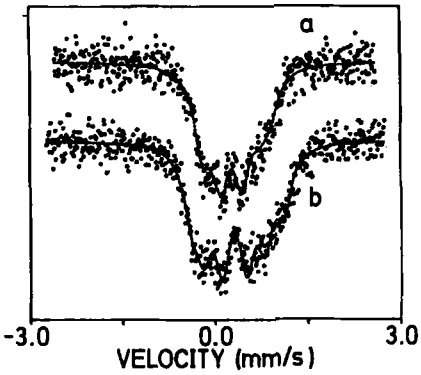

FIG. 6 Transmission spectra of $Fe_{1.25}Nb_{2.75}Se_{10}$ (a) and of $Fe_{1.33}Ta_{0.67}Nb_2Se_{10}$ (b)

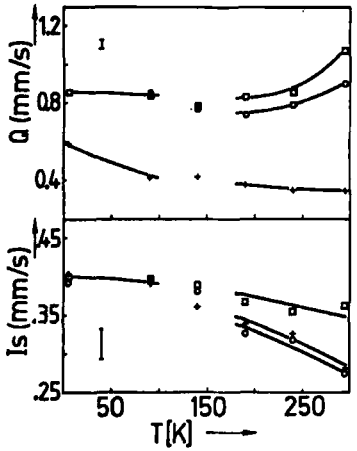

FIG.7 Temperature dependence of Q and Is for $Fe_{1.25}Nb_{2.75}Se_{10}$ intensities for the subspectra .21 (□), .22(o), .57(+), (see FIG. 5b)

T<140 K only minor differences of Is were measured and Q for the two subspectra representing Fe mainly surrounded by Nb coincide, whereas Q for Fe mainly surrounded by Fe is still different and exhibits a distinct temperature dependence. From the behaviour of Q a strong distortion of the charge density of Fe caused by the surrounding Nb is suggested.

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