Nuclear magnetic resonance of ^{119}Sn, ^{95}Mo, and ^{33}S in the compound $SnMo_6S_8$

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The results are reported of measurements of the magnetic susceptibility and of the NMR spectra of ^{95}Mo, ^{119}Sn, and ^{33}S in the normal and superconducting states of the compound $SnMo_6S_8$ which has the Chevrel phase structure. A combined analysis of the results is used to separate the contributions made to the magnetic susceptibility and to analyze the nature of the electron states near the Fermi level. The possibility of the presence of inequivalent positions of the tin atoms in this compound is considered.

INTRODUCTION

The compound $SnMo_6S_8$ belongs to the currently very topical class of superconducting ternary molybdenum chalcogenides (TMCs) with the Chevrel phase structure.[1,2] The crystal structure of the Chevrel phases is rhombohedral ($R\bar{3}$ symmetry) and can be regarded as consisting of Mo_6S_8 blocks with atoms of the third component located in channels between these blocks. In the case of $SnMo_6S_8$ the rhombohedral angle α is close to 90° and the tin atoms are located at the (0,0,0) positions forming an almost-cubic lattice.[3,4]

The temperature of the superconducting transition in $SnMo_6S_8$ reaches 14 K and the derivative of the second critical magnetic field near T_c is ~ 37 kOe/K (Ref. 2). Measurements of the specific heat have shown that the coefficient γ of this compound is 84 $mJ \cdot mol^{-1} \cdot K^{-2}$ (Ref. 5), indicating that the density of states at the Fermi level is high. An estimate of the density of states can, in principle, be obtained also from the magnetic susceptibility χ. However, we must bear in mind that the susceptibility may include not only the Pauli but also other contributions. A correlation between the temperature dependences of the Knight shift of ^{119}Sn and of the magnetic susceptibility of $SnMo_6S_8$ is used in Ref. 6 to propose the hypothesis that the main contribution to the susceptibility of this compound is of the Pauli origin. A detailed analysis of the contributions made to the magnetic susceptibility can be carried out on the basis of a combined analysis of the susceptibility data and of the NMR spectra of the nuclei of the transition element with electron states which are assume to make a considerable contribution to the density of state $N(0)$ at the Fermi level. It would be if interest to carry out also NMR investigations of the nuclei of other atoms in this compound in order to identify their role in the formation of the density of states at the Fermi level. Moreover, such NMR investigations may help in identifying features of the structure of this compound.

We shall report the results of an investigation of the magnetic susceptibility, nuclear magnetic resonance, and spin-lattice relaxation of the ^{95}Mo, ^{119}Sn, and ^{33}S nuclei in $SnMo_6S_8$ in the normal and superconducting states. We shall discuss the relationship between the results obtained, on the one hand, and the electron and structure characteristics of the investigated compound, on the other.

SAMPLES AND INVESTIGATION METHOD

Samples of ternary tin molybdenum sulfide were prepared from the three components enriched with the ^{95}Mo, ^{119}Sn, and ^{33}S isotopes employing a synthesis technology described in Ref. 5. We used samples *A*, *B*, and *C* with the structure and superconducting characteristics listed in Table I. We also included in Table I the results of an activation analysis of the iron content c_{Fe} in these samples; the influence of iron on T_c had been investigated in detail earlier.[7] Sample *C* was prepared from the original sample, with characteristics similar to those of sample *A*, by annealing in a

TABLE I. Properties of investigated samples.

Compound	$SnMo_6S_8$		
Sample	A	B	C
Isotopic enrichment	^{33}S, ^{95}Mo, ^{119}Sn	^{119}Sn	–
T_c, K	11.5	12.8	14.1
c_H, A	11.356 ∓ 0.003	11.378 ∓ 0.003	11.377 ∓ 0.003
a_H, Å	9.176 ∓ 0.003	9.181 ∓ 0.003	9.183 ∓ 0.003
V_H, Å^3	828.0 ∓ 0.8	830.6 ∓ 0.8	830.8 ∓ 0.8
c_{Fe}, at.%	0.017	0.009	–
$I_2/(I_1+I_2)$ $(T=300$ K)	0.24	0.20	0.17
$I_2/(I_1+I_2)$ $(T=16$ K)	0.10	0.05	0.00

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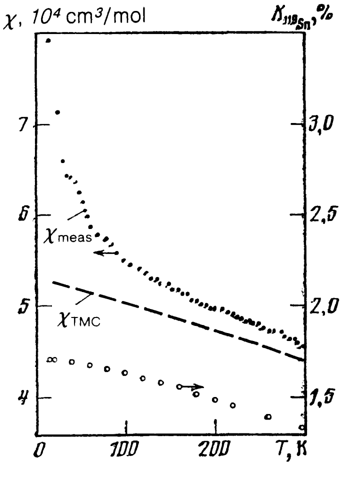

FIG. 1. Temperature dependences of the magnetic susceptibility of $SnMo_6S_8$ characterized by $T_c = 11.5$ K (χ_{meas}), of the magnetic susceptibility corrected to allow for the concentration of atomic iron in this compound (χ_{TMC}), and of the Knight shift of ^{119}Sn in type A sample.

hydrogen atmosphere ($p_H = 760$ Torr for 5 h at $T = 825 \pm 25$ °C). After annealing in this hydrogen atmosphere the superconducting transition temperature T_c rose to 14.1 K, but the width of the superconducting transition increased to 0.8 K.

The samples usually had a small excess of tin, so that the x-ray diffractograms included weak lines of β-Sn. The NMR signal of this phase was used as a comparison standard in the determination of the ^{119}Sn signal obtained for $SnMo_6S_8$.

The NMR experiments were carried out in the temperature range 4–300 K using an SXP 4-100 spectrometer made by Bruker; they were carried out at frequencies of 2.9, 5.64, 13 MHz (^{95}Mo); 5.64 and 32.5 MHz (^{119}Sn), and 5.64 MHz (^{33}S) employing an electromagnet and a superconducting magnetic system. The spin-lattice relaxation time T_1 was measured by recording the amplitude of the spin echo signal when the delay τ between the saturating sequence and a pair of rf pulses forming the echo was varied. Recovery of the magnetization $M_z(\tau)$ was described satisfactorily by the dependence $1 - \exp(-\tau/T_1)$ with one characteristic time (for $\tau > T_1$). The amplitude of the circular component of the rf field (H_1) reached 70 Oe. The NMR spectra of ^{95}Mo, ^{33}S, and ^{119}Sn were recorded by the method of hf phase detection of the spin echo signal followed by its analog integration. The signal/noise ratio was increased by repeated recording of the spectrum and accumulating the results in the memory of an Élektronika D3-28 microcomputer. The shifts of the resonance lines of ^{95}Mo, ^{33}S, and ^{119}Sn were determined employing a tracking NMR gaussmeter and the following values of the gyromagnetic ratio: $(\gamma/2\pi)_{^{95}\mathrm{Mo}} = 277.4$ Hz/Oe, $(\gamma/2\pi)_{^{33}\mathrm{S}} = 326.54$ Hz/Oe, $(\gamma/2\pi)_{^{119}\mathrm{Sn}} = 1586.9$ Hz/Oe. The shifts of the lines of the tin and sulfur nuclei were deduced from the positions of the maxima of the absorption lines. Components of the Knight shift tensor of ^{95}Mo were determined from an analysis of the field dependences of the profile of the central transition line ($-\frac{1}{2} \leftrightarrow \frac{1}{2}$) in accordance with Ref. 8. Since the quadrupole satellite singularities were strongly broadened, only an estimate could be obtained of the quadrupole coupling constant of ^{95}Mo: $\nu_Q(SnMo_6S_8) = 115 \pm 10$ kHz.

The magnetic susceptibility was determined by the Faraday comparison method using an electronic microbalance with automatic compensation. The error in the relative values of χ did not exceed 0.01, whereas the error in the absolute value was not more than 0.05χ. A molybdenum single crystal, assumed to have the susceptibility $\chi(300\ \mathrm{K}) = 82.5 \times 10^{-6}$ cm^3/mol, was used as a reference standard.

EXPERIMENTAL RESULTS

Figure 1 shows the temperature dependence of χ for sample A with $T_c = 11.8$ K in which all three nuclei were isotopically enriched. The NMR data for this sample were used later to analyze the contributions made to the magnetic susceptibility. The absolute value of χ at room temperature obtained by us was slightly higher than that given in Ref. 1. The observed increase in the slope of the temperature dependences below 80 K was due to the presence of a small number of impurities in the original molybdenum. We therefore found

$$\chi_{\mathrm{meas}} = \chi_{\mathrm{TMC}} + \chi_{\mathrm{imp}} \qquad (1)$$

The results of the activation analysis (Table I) showed that the concentration of the ion atoms in this sample was approximately 0.017 at.%. Bearing in mind that in this range or iron concentrations the impurity has a magnetic moment $\mu_{\mathrm{Fe}} = 4\mu_B$ (Ref. 9), we can subtract the impurity contribution χ_{imp} and thus determine more accurately the behavior of the susceptibility of the ternary molybdenum chalcogenide χ_{TMC} at low temperatures (dashed curve in Fig. 1). This temperature dependence of χ_{TMC} agreed well, within the limits of the experimental error of χ, with the results of Ref. 10.

Figure 2 shows the temperature dependences of the components of the Knight shift tensor of the ^{95}Mo nuclei: the isotropic (K_{iso}) and anisotropic (K_{ax}) components are given for sample A. The Knight shift data differ from those given in Ref. 11, where it is reported that the value $K_{\mathrm{Mo}} = 1.55\%$ is temperature-independent. The values of $(T_1T)^{-1}$ for ^{95}Mo are plotted as a function of temperature in Fig. 3. It is worth noting the reduction in the slopes fof the temperature dependences of K_{ax}, K_{iso}, and $(T_1/T)^{-1}$ below

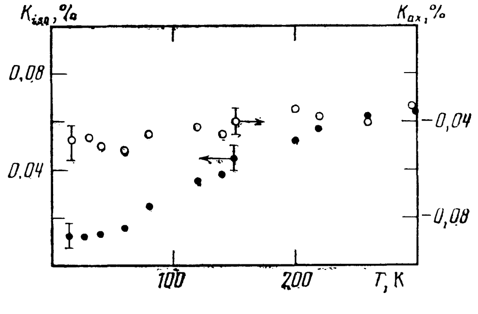

FIG. 2. Temperature dependences of the isotropic (K_{iso}) and anisotropic (K_{ax}) components of the Knight shift tensor of ^{95}Mo of a sample of type A.

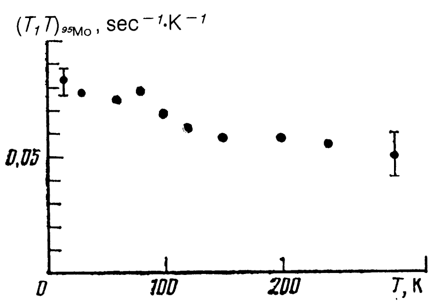

FIG. 3. Temperature dependence of $(T_1T)^{-1}$ obtained for ^{95}Mo in a sample of type A.

100 K. Such weakening of the temperature dependences applies also to the Knight shift of ^{119}Sn (Fig. 1), which is reported in Ref. 6, and to the value of $(T_1T)^{-1}$ (Fig. 4). The Korringa ratio T_1TK^2 for ^{119}Sn remains practically constant in the range of temperatures corresponding to the existence of the normal state.

The transition to the superconducting state reduces the Knight shift of ^{119}Sn from 1.72% ($T = 14$ K) to 1.35% of $T = T_c/2 = 6$ K. This result indicates a nonzero density of states of tin at the Fermi level in the investigated ternary molybdenum sulfide. A similar conclusion follows also on the role of states of the sulfur atoms. The sulfur nuclei are characterized by a negative Knight shift $K_{^{33}\mathrm{S}} = -0.2\%$. The rate of relaxation of ^{33}S in the normal state up to $T = 60$ K is proportional to temperature, within the limits of the experimental error, and it is given by $(T_1T)^{-1} = 0.038 \pm 0.005$ sec^{-1}·K^{-1}. An estimate of the Korringa ratio gives $(T_1TK^2)_{^{33}\mathrm{S}} = 1.4 \times 10^{-4}$ sec·K. A finite density of the tin sulfur states at the Fermi level is manifested most clearly in the behavior of the rate of the spin-relaxation of the ^{33}S and ^{119}Sn nuclei in the superconducting state of the compound. The appearance of an energy gap should in this case increase exponentially the spin-lattice relaxation time of the nuclei of those atoms which contribute electrons to the formation of Cooper pairs. Figure 5 shows the dependence of $T_1(T)/T_1(T_c)$ on (T_c/T) for all three investigated nuclei. It is clear from this figure that the experimental points are described satisfactorily by an exponential dependence. It follows that the main spin-lattice relaxation mechanism of all three types of nuclei is associated with the appearance of a superconducting gap. The absence of a discontinuity of T_1 at the point $T = T_c$ is typical of the spin-lattice relaxation processes in superconductors in the "dirty" limit. An estimate of the energy gap from these data gives $2\Delta/k_BT_c \approx 4.5$, which is close to the value obtained from an analysis of the specific heat.[5]

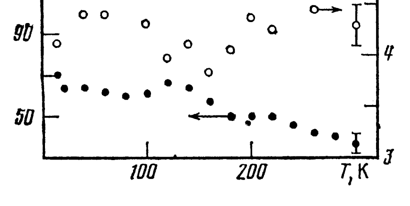

FIG. 4. Temperature dependences of $(T_1T)^{-1}$ and K^2T_1T obtained for ^{119}Sn in a sample of type A.

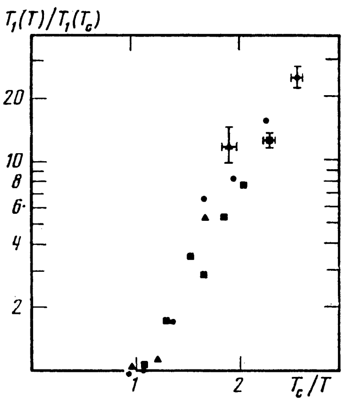

FIG. 5. Dependence of $T_1(T)/T_1(T_c)$ on the relative value of the reciprocal of temperature below T_c for a sample of type A: ●) ^{95}Mo; ■) ^{119}Sn; ▲) ^{33}S.

Evolution of the NMR spectra of ^{119}Sn due to variation of the temperature of samples with different values of T_c is demonstrated in Fig. 6. The NMR spectra of ^{119}Sn of all three samples consist of the following three lines:

1) the strongest line with the behavior of the Knight shift and the spin-lattice relaxation discussed above;

2) a line with a temperature-independent Knight shift $K = 0.90 \pm 0.01\%$; on transition to the superconducting state the shift of this line decreases to $0.86 \pm 0.03\%$ at $T = 6$

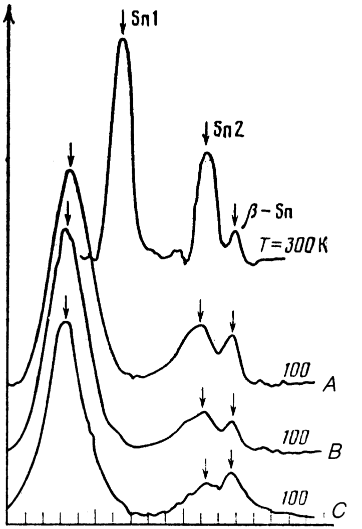

FIG. 6. Spectra of ^{119}Sn obtained for SnMo$_6$S$_8$ samples with different values of T_c at the frequency $\nu = 32.703$ MHz.

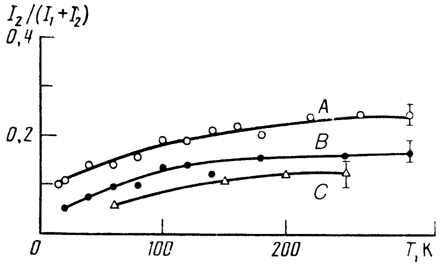

FIG. 7. Temperature dependences of the relative intensity of line 2 obtained for $SnMo_6S_8$ samples with different values of T_c.

K, which is considerably less than the corresponding change in Knight shift of line 1;

3) a line with a temperature-independent Knight shift $K_{Sn} = 0.72 \pm 0.01\%$, corresponding to metallic β-Sn.

Lines 1 and 2 have similar profiles and the same width. Moreover, the increase in the line width as a result of cooling is the same. The frequency dependence of the line width shows the inhomogeneous broadening occurs because of the distribution of the Knight shift of the tin nuclei. An additional confirmation of the inhomogeneous nature of the broadening is the behavior of the spin-lattice relaxation time T_2 of the ^{119}Sn nuclei for line 1. At temperatures above 60 K the amplitude of the spin echo signal decays exponentially with a time constant T_2 approaching the spin-lattice relaxation time T_1. Below 60 K the decay of the echo amplitude becomes Gaussian, indicating the appearance of a magnetic inequivalence (within the limits of the line width) of the nearest tin atoms in the structure of $SnMo_6S_8$. The behavior of T_2 for line 2 is qualitatively the same, but the error in the time measurements is considerably greater.

The combined intensity of the first and second lines $(I_1 + I_2)$ was determined relative to the intensity of the β-Sn line and it was found that it remained constant throughout the investigated temperature range within the limits of the error (~ 0.05). The behavior of the relative intensity of the second line $I_2/(I_1 + I_2)$ is demonstrated in Fig. 7. It is worth noting the parallel shift of the curves representing different samples. A redistribution of the line intensities on increase in temperature is of the thermally activated type with an activation energy $E_a \approx 300 \pm 50$ K. These observations allow us to postulate the existence of inequivalent (in the magnetic sense) positions of the tin atoms Sn1 and Sn2, and a correlation of the low-temperature population at the position Sn2 with the value of T_c.

DISCUSSION OF RESULTS

It is known that the magnetic susceptibility of ternary molybdenum chalcogenides χ_{TMC} can be represented in the form of the following contributions: the diamagnetic susceptibility of the ionic cores χ_{dia}, the spin susceptibilities of the electrons in the d and s bands χ_d and χ_s, and the Van Vleck susceptibility of the d electrons χ_{orb}:

$$\chi=\chi_{dia}+{}^2/{}_3\chi_s+\chi_{orb}+\chi_d. \tag{2}$$

The coefficient 2/3 in front of χ allows for the contribution of the Landau diamagnetism to the susceptibility of the s electrons. In the case of $SnMo_6S_8$ we have $\chi_{dia} = 3.6 \times 10^{-4}$ cm^3/mol (Ref. 12). The other contributions can be separated using the data on the magnetic resonance and relaxation of the ^{95}Mo nuclei.

In the tight-binding approximation in the case of the d electrons, allowing for the symmetry of the immediate environment C_{4v} of the molybdenum atoms, we find that the components of the Knight shift tensor and of $(T_1T)^{-1}_{Mo} = R$ can be represented similarly in the form of sums of the following main terms[13]:

$$K_{iso}(\mathrm{Mo})=\frac{1}{\mu_B}[H_s\chi_s+H_{orb}\chi_{orb}-|H_d|\chi_d(T)], \tag{3}$$

$$K_{ax}(\mathrm{Mo})=\frac{1}{7\mu_B}H_{orb}\chi_d(T)r+K_{ax}^{orb}, \tag{4}$$

$$R_{\mathrm{Mo}}=R_s+R_d(T)=2\gamma_{\mathrm{Mo}}{}^2hk_BH_s{}^2N_s{}^2+2\gamma_{\mathrm{Mo}}{}^2hk_B \times\left(\frac{\chi_d}{2\mu_B}\right)^2\left(H_d{}^2p+H_{orb}^2\frac{2\mu_B{}^2}{2\mu_B{}^2+J\chi_d{}^2}q\right); \tag{5}$$

where H_s, H_d, and H_{orb} are the hyperfine fields at the molybdenum nuclei created by the spin moment of the electrons in the s and d bands, and by the orbital moment of the electrons from the d band: $H_s = 2.72 \times 10^6$ Oe, $H_{orb} = 0.3 \times 10^6$ Oe (Ref. 14). The slope of the dependence $K_{iso}(\chi)$ gives $H_d = -2.6 \times 10^5$ Oe, which is close to that used in Ref. 14 for metallic molybdenum; N_s and N_d are the densities of states of the Fermi level in the s and d bands.

The value of R is proportional to the square of the density of the states and depends on the ratio of the weights $(f_i = N_i/N_0)$ of the d states of different angular symmetries at the Fermi level. When an allowance is made for the nearest neighbors of the molybdenum atom, the d band can be regarded as consisting of four subbands, which are formed by the d_z^2 (σ subband), d_{zx}, d_{zy} (π subband), d_{xy} (δ_1 subband), and $d_{x^2-y^2}$ (δ_2 subband) states; the z axis is directed along the C_4 axis in the local coordinate system linked to the molybdenum atom. In this case the coefficients p, q, and r allow for the influence of the degree of degeneracy of the states in the d band, which can be described as follows:

$$p=f_\sigma{}^2+0.5f_\pi{}^2+f_{\delta_1}{}^2+f_{\delta_2}{}^2, \tag{6a}$$

$$q=1.5f_\pi f_\sigma+0.5f_\pi f_{\delta_1}+0.5f_\pi f_{\delta_2}+0.25f_\pi{}^2+f_{\delta_1}{}^2+f_{\delta_2}{}^2, \tag{6b}$$

$$r=f_\sigma+0,5f_\pi-f_{\delta_1}-f_{\delta_2}. \tag{6c}$$

We used the above assumptions in estimating the contributions made to the magnetic susceptibility of the compound $SnMo_6S_8$. The various contributions were found by successive approximations. We first estimated χ_S from the relationship $R_{exper} = R_s$. We then used Eqs. (2) and (3) for selected values of H_d and H_{orb} and found the orbital and spin contributions of the d electrons, and finally obtained a more accurate value of the spin susceptibility of the s-band electrons using the dependence $R(\chi_d^2)$. Table II gives the results of our separation of the contributions to the magnetic susceptibility and the Knight shift at $T = 80$ K, where the impurity contribution to χ_{meas} is small. The change in χ_{TMC} as a result of cooling from 80 K to T_c is slight, so that the values given in Table II reflect the ratio of the contributions also at lower temperatures. The main error in this procedure

TABLE II. Results of separation of contributions to magnetic susceptibility of $SnMo_6S_8$ sample A ($T_c = 11.5$ K) at $T = 80$ K.

$\chi_{dia}\cdot 10^4$, cm^3/mol	$\chi_d\cdot 10^4$, cm^3/mol	$\chi_{orb}\cdot 10^4$, cm^3/mol	$\chi_s\cdot 10^4$, cm^3/mol
−3.6	4.5∓0.5	4.1∓0.5	0.1
K_s, %	K_{orb}, %	K_d, %	$(T_1T)^{-1}$, с$^{-1}$·К$^{-1}$
0.03	0.33∓0.04	−0.34∓0.04	0.02

of separation of the contributions comes from some indeterminacy of the selection of $H_{\rm orb}$, the values of which depend on the spatial extent of the *d* orbitals in the compound. The field $H_{\rm orb} = 300$ kOe is taken from the paper of Narath and Alderman[14] and it applies to metallic molybdenum. Following Ref. 14, we can assume that the change in $H_{\rm orb}$ in the compound does not exceed a factor of 2 and this determines the error in the estimates of $\chi_{\rm orb}$ and χ_d listed in Table II.

The main contribution to the magnetic susceptibility of $SnMo_6S_8$ comes from the spin paramagnetism of the 4*d* electrons of molybdenum. The orbital contribution is largely compensated by the diamagnetism of the compound, as assumed in Ref. 6. The result can be regarded as justification for the estimates of the density of states in ternary molybdenum chalcogenides based on the measured value of the magnetic susceptibility.

If the density of states is high, then an estimate of $N(0)$ from χ_d must allow for the exchange enhancement:

$$N(0) = \chi_d/(2\mu_B^2 + J\chi_d), \tag{7}$$

where J is the exchange intergral. The exchange integral of the Chevrel phases used in Ref. 15 is $J = 0.54$ eV and it is obtained by calculation from metallic molybdenum. An estimate of the one-particle density obtained using this value of J is $N(0) = 0.8 \pm 0.2$ eV^{-1} (Mo atom)$^{-1}$·spin^{-1} and it is in satisfactory agreement with an estimate deduced from measurements of the specific heat allowing for the electron-phonon interaction constant of $SnMo_6S_8$ (Ref. 5).

The correlation between the temperature dependences of the Knight shift of ^{119}Sn and of the magnetic susceptibility and the behavior of the Knight shift of ^{119}Sn and of the spin-lattice relaxation times of ^{119}Sn and ^{33}S in the superconducting state suggests that a nonzero density of the electron states of tin and sulfur may exist at the Fermi level. One of the possible reasons for this may be hybridization of the electron states of molybdenum with the states of tin and sulfur near the Fermi level. This is not in conflict with the results of calculations of the electron spectrum from first principles.[16] The conclusions reached in the cited papers on the nature of states of the sulfur and tin atoms at the Fermi level are in qualitative agreement with our results.

We can estimate the exchange integral J from our values of the Korringa ratio for tin and sulfur on the assumption that the Knight shift and the spin-lattice relaxation of the nuclei are of spin origin. The most probable reason for the discrepancy between the experimental and theoretical values of the Korringa ratio is the influence of the collective electron effects on the Knight shift and on the spin-lattice relaxation rate:

$$T_1TK^2 = \left(\frac{2\pi\gamma_{\rm Sn}^2 h k_B}{4\mu_B^2}\right)\{k\,[JN(0)]\}^{-1}. \tag{8}$$

In the case of a free electron gas we have $k = 1$. An increase in the influence of the collective effects reduces $k[JN(0)]$ and increases the observed Korringa ratio. We can estimate integral J using the expression for $k[JN(0)]$ obtained in the Fermi-liquid approximation for a near-spherical Fermi surface.[13] It follows from the data for ^{119}Sn that $J = 0.45 \pm 0.07$ eV, whereas the data for ^{33}S give the exchange integral $J = 0.43 \pm 0.1$ eV, which is close to the value used above for metallic molybdenum. These values improve the agreement between the estimates of $N(0)$ deduced from the NMR data and those given in Ref. 5.

We have pointed out above (Fig. 2) that $K_{\rm ax}$ for ^{95}Mo is negative. The negative value of $K_{\rm ax}$ for ^{95}Mo [Eqs. (4) and (6)] is possible only when the states in the δ subbands at the Fermi level dominate the total density of states. The spin-lattice relaxation data for the ^{95}Mo nuclei can be used to obtain a quantitative estimate of the range of possible values of the relative contribution of states of this type of symmetry:

$$0.6 < f_{\delta_1} + f_{\delta_2} < 0.8. \tag{9}$$

The presence of the two lines Sn1 and Sn2 in the spectrum of ^{119}Sn may be attributed to the existence of inequivalent positions of tin in the $SnMo_6S_8$ structure. However, one of the probable reasons for such inequivalence may be the presence of oxygen atoms in the $SnMo_6S_8$ compound, as discussed in Ref. 17. The structure data are used in Ref. 17 to conclude that the inequivalent tin positions may appear because of the displacement of the Sn atoms along the C_3 axis toward the oxygen atoms occupying the sulfur positions S2. A correlation between the value of T_c and the hexagonal parameters of the unit cell of $SnMo_6S_8$ containing oxygen is also established in Ref. 17. Our results also indicate a correlation between the intensity of the second line, on the one hand, and T_c and the structure parameters, on the other (Table I). However, we cannot exclude another probable explanation involving possible structure distortions in the $SnMo_6S_8$ lattice.[18,19] Such distortions may be responsible for the observed redistribution of the intensities of the Sn1 and Sn2 lines (Fig. 7). It should be pointed out that the observed thermally activated process differs from the usual chemical exchange of tin atoms between different positions, as postulated in Ref. 6 in connection with an analysis of the narrowing of line 1 on increase in temperature. Clearly, we are dealing here with a thermodynamic-equilibrium (at a given temperature) ratio of the populations of tin at two inequivalent positions.

The fact that the Knight shift of Sn2 is independent of temperature and changes only slightly on transition to the superconducting state may indicate that the contribution of the tin atoms in this position to the density of states at the Fermi level is small. However, the true reason for the appearance of the Sn2 line will require further studies of the structure.

CONCLUSIONS

A combined analysis of the temperature dependences of the magnetic susceptibility, of the isotropic Knight shift of ^{95}Mo, and of the rate of the spin-lattice relaxation of ^{95}Mo in the compound $SnMo_6S_8$ is used to estimate the main contributions to the susceptibility of this compound. The results confirm an earlier hypothesis that the susceptibility is dominated by the Pauli contribution of the $4d$ electrons of molybdenum. The orbital and diamagnetic contributions largely balance out each other. The Pauli contribution including the exchange enhancement is used to estimate the density of electron states at the Fermi level in the compound $SnMo_6S_8$: $N(0) = 0.8 \pm 0.2$ eV·(Mo atom)$^{-1}$·spin^{-1}. The negative sign of the anisotropic shift of ^{95}Mo in this compound suggests that the greatest contribution to $N(0)$ comes evidently from the $4d$ states of molybdenum with the $d_{x^2-y^2}$ and d_{xy} symmetries. The temperature dependences of the spin-lattice relaxation rate obtained for the ^{95}Mo, ^{119}Sn, and ^{33}S nuceli below T_c gives $2\Delta/k_B T_c \approx 4.5$, confirming the strong binding in the $SnMo_6S_8$ compound in the superconducting state. The NMR spectrum of ^{119}Sn in $SnMo_6S_8$ has an additional line which may be attributed to a further inequivalent position of tin. A correlation established between the intensity of this line and the value of T_c shows that one of the possible reasons for the appearance of such an equivalent position may be the presence of defects in the structure of the investigated compound.

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