

probe particles which do not affect the magnetic state of a layer of chemisorbed carbon monoxide molecules.

The results obtained by us show that the thermomagnetic effect can be used to study the magnetic properties of monolayers of chemisorbed particles.

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Nuclear magnetic resonance of ^{51}V in a V_3Si single crystal above and below the structural transition temperature

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We investigated the temperature dependences of the Knight shift, of the quadrupole-interaction constant, and of the spin-lattice and spin-spin relaxation times of ^{51}V nuclei, and also of the magnetic susceptibility in single-crystal V_3Si in the normal state. All the measured quantities with the exception of the spin-lattice relaxation time have singularities near the structural phase-transition temperature $T_M = 21$ K. As T_M is approached from above, a pretransition broadening of the quadrupole satellites is observed and is attributed by us to statistical distortions of the lattice near the defects. The hyperfine magnetic fields at the ^{51}V nuclei and the contributions of the wave functions of various symmetry to the density of the electronic states on the Fermi level are determined from the experimental data. The main contribution to the state density on the Fermi level is made by π -symmetry states.

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The intermetallide V_3Si , which has a crystal structure of the A-15 type, has unusual electron and phonon properties.¹ Particular interest attaches to the existence in V_3Si of a structural cubic to tetragonal phase transition at the point of the martensitic transition $T_M \approx 21$ K. In a number of theoretical models proposed to explain the anomalous properties of compounds of the A-15 type²⁻⁴ it is assumed that the Fermi level passes near the narrow peak of the density of the electronic states, and the structural transition is attributed to instability of the electronic structure. At the present time, however, experimental data exist and make it possible to determine uniquely the details of the band structure of these compounds. It is therefore of interest to perform ex-

periments that yield information on the electronic structure of V_3Si and on the character of its variation in phase transitions. This information can be obtained with the aid of nuclear magnetic resonance (NMR).

The NMR parameters are most sensitive to changes of the density of the electronic states on the Fermi level $N(E_F)$ and the symmetry of the nearest environment of the investigated nuclei. Direct information on the variation of $N(E_F)$ can be obtained also from measurements of the magnetic susceptibility χ , the results of which supplement the NMR data. A maximum of χ is observed at the temperature of the structural transition in V_3Si single crystals.⁵ A splitting of the spectral

lines of polycrystalline V_3Si in the structural transition was observed in Refs. 6 and 7 and was attributed to the existence of two nonequivalent positions on the vanadium atoms in the tetragonal phase. However, the NMR parameters determined from the spectra is not always single-valued in the case of polycrystals. An investigation of single-crystal samples permits a more reliable determination of the NMR parameters and of their anisotropy. The orientation dependence of the NMR spectra in the V_3Si single crystal was investigated at 77 K (Ref. 8) and at room temperature.⁹ The V_3Si single crystal was investigated also by the method of nuclear acoustic resonance (NAR) at 77 and 17 K.¹⁰

We report here an investigation of the temperature dependence of the stationary (Knight shift, quadrupole-interaction constant) and nonstationary (spin-lattice and spin-spin relaxation times) parameters of the NMR of ^{51}V and of the magnetic susceptibility in the single crystal V_3Si . We discuss the behavior of the characteristics of the NMR near the structural-transition temperature and the nature of the pretransition phenomena in V_3Si . A joint analysis of the temperature dependences of the NMR parameters and of the magnetic susceptibility as enabled us to determine the hyperfine magnetic fields at the ^{51}V nuclei and the contributions of the electronic states of different symmetry to $N(E_F)$.

EXPERIMENTAL PROCEDURE

The V_3Si single crystal was grown at the Institute of Solid State Physics of the USSR Academy of Sciences by a method described in Ref. 8. The crystal was a parallel-piped with dimensions $13 \times 9 \times 5$ mm. It was cut into platelets 0.2 mm thick parallel to the (001) plane. The superconducting transition temperature was 16.4 K, the lattice parameter was 4.725 ± 0.001 Å, and the resistance ratio was $\alpha_R \equiv R(300 \text{ K})/R(17 \text{ K}) = 45$.

The NMR measurements were made with a Brooker pulsed coherent spectrometer SXP 4-100 at a frequency $\nu = 12$ MHz. The NMR spectrum was recorded by integrating the free-precession fall-off signal with simultaneous scanning of the magnetic field. The magnetic field H was parallel to the [001] axis when the spectra were recorded. The spin-lattice and spin-spin relaxation times T_1 and T_2 were measured under the conditions of the "magnetic angle" ($H \parallel [111]$). At this field orientation the Zeeman levels are equidistant in first order in the quadrupole interaction, and a single narrow line is observed instead of the complex spectrum, so that it is possible to measure T_1 by using a simple two-pulse $90^\circ - 90^\circ$ sequence; the time T_2 was determined by measuring the damping of the echo signal with increasing interval between the two RF pulses. To increase the signal/noise ratio we accumulated the periodically repeated signal in a computer. The magnetic susceptibility was measured by the relative Faraday method with the aid of an electron balance with automatic compensation.

The temperature of the sample placed in an evaporation helium cryostat was monitored against a carbon resistor calibrated with a standard platinum thermome-

ter. The temperature stability during the measurement time was not worse than 0.03 K.

EXPERIMENTAL RESULTS AND THEIR DISCUSSION

1. The NMR spectrum

The vanadium nuclei in the A-15 structure are in positions with tetragonal symmetry D_{2d} . The noncubic symmetry of the environment leads to a splitting of the ^{51}V resonance line on account of the interaction between the electric quadrupole moment of the nucleus and the gradient of the local electric field. The resonant magnetic fields corresponding to transitions with change of the magnetic quantum number $m \leftrightarrow m - 1$ are determined, accurate to second order perturbation theory in the quadrupole interaction, by the expression¹¹

$$H_{m \leftrightarrow m-1} = (1+K)^{-1} \left[H_0 - \frac{1}{2} H_Q \left(m - \frac{1}{2} \right) (3 \cos^2 \theta - 1) + \eta \sin^2 \theta \cos 2\varphi \right] - \frac{H_Q^2}{32H_0} S_m(\theta), \quad (1)$$

$$K = K_{iso} + K_{ax} (3 \cos^2 \theta - 1), \quad H_Q = \frac{2\pi}{\gamma} \frac{3e^2qQ}{2hI(2I-1)},$$

$$S_m(\theta) = \sin^2 \theta \{ [102m(m-1) - 18I(I+1) + 39] \cos^2 \theta - [6m(m-1) - 2I(I+1) + 3] \}.$$

Here I is the nuclear spin ($I = 7/2$ for ^{51}V), γ is the gyromagnetic ratio of the nucleus, eQ is the quadrupole moment of the nucleus, eq is the maximum principle value of the electric field gradient (EFG) tensor at the location of the nucleus, e is the electron charge, h is Planck's constant, θ and φ are the polar and azimuthal angles of the direction of the magnetic field in the system of the principal axes of the EFG tensor, η is an asymmetry parameter that characterizes the deviation of the EFG from axial symmetry, $H_0 = 2\pi\nu/\gamma$ is the resonant field of ^{51}V in the diamagnetic salt, and K_{iso} and K_{ax} are the isotropic and anisotropic components of the Knight shift.

It was shown in Ref. 8 that the EFG tensor and the Knight shift in V_3Si have axial symmetry ($\eta = 0$) with a symmetry axis directed along the vanadium-atom chains (type [100] direction). Since V_3Si has three mutually perpendicular systems of vanadium chains, the angle θ in (1) assumes, at an arbitrary magnetic-field orientation, three different values, and the NMR spectrum is a superposition of three uniaxial spectra. At $H \parallel [001]$, a superposition of two spectra is observed corresponding to the angles 0 and 90° (total of 14 lines). At $H \parallel [111]$, $3 \cos^2 \theta - 1 = 0$ for all chains and, according to (1), there is no quadrupole splitting in first order. In this case a single line was observed in the spectrum.

2. Pretransition phenomena

The NMR line width remains unchanged when the temperature is lowered from 77 to 35 K. With further approach to T_M , an appreciable broadening of the quadrupole satellites is observed (Fig. 1). Since the local EFG is quite sensitive to changes of the symmetry of the nearest invariant of the vanadium atoms the broadening of the satellites can be connected with fluctuating or static changes in the local symmetry.

The observed broadening of the NMR lines can be re-

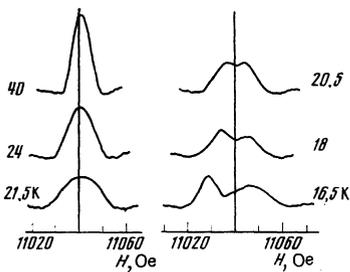


FIG. 1. Evolution of the NMR line of ^{51}V corresponding to the transition $m = 5/2 \rightarrow 7/2$ ($\theta = 90^\circ$), in V_3Si with changing temperature.

garded as a manifestation of the pretransition "central peak," the nature of which is presently discussed in the literature.¹² Two mechanisms leading to the appearance of the central peak have been proposed¹²: fluctuations of the order parameter, and onset of local order near defects ("phase transition in defects") above the phase-transition point in the entire volume of the sample. The first mechanism should lead to a homogeneous broadening of the NMR lines and to an appreciable decrease of T_2 near T_M . The second mechanism, however, should lead to an inhomogeneous broadening of the lines, and consequently should not exert a substantial influence on T_2 . Measurements have shown that the time T_2 remains approximately constant in the temperature interval 17–77 K and is equal to 120 ± 10 μsec . This result leads to the conclusion that the observed pretransition broadening of the lines is inhomogeneous and is due not to dynamic structural fluctuations, but to static lattice distortions which apparently arise near the defects. Thus, our data agree qualitatively with the Phillips model,¹³ which emphasizes the role of defects as centers of nucleation of the tetragonal phase in V_3Si above T_M . Favoring the existence of tetragonal-phase microdomains above T_M are also a number of other experimental facts, particularly ultrasound second-harmonic generation,¹⁴ which is forbidden by cubic symmetry, and an anomalous behavior of the coefficient of thermal expansion in V_3Si .^{15,16}

We note that the conclusion that static displacements of the atoms take place in V_3Si above T_M does not contradict the available data on the "softening" of the lattice, inasmuch as in the pretransition region the central peak can coexist with softening of the phonon modes. Moreover, static displacements become possible with apparently only in the case of a sufficiently strong "softening" of the lattice. The phonon frequencies, however, remain too large to influence the width of the NMR lines.

3. Quadrupole interaction

The quadrupole interaction constant $V = e^2qQ/h$ was determined from the NMR spectrum with the aid of relation (1). In the temperature interval from $T_M = 21$ to 77 K the value of V remained constant at $V = 2.84 \pm 0.01$ MHz. This value is close to the result given in Ref. 8 (2.870 ± 0.014 MHz), but is somewhat less than the value of V obtained by the NAR method¹⁰ (2.92 ± 0.02 MHz) at 77 K.

TABLE I.

	V_c , MHz	V_a , MHz	$V_c - V_a$, MHz	η_a
Present work (16,8 K)	2.890 ± 0.010	2.583 ± 0.010	0.307	0.015 ± 0.010
Ref. 10 (17 K)	3.240 ± 0.030	2.975 ± 0.060	0.265	0.12 ± 0.03

A temperature dependence of the splitting of the quadrupole satellites (Fig. 1) was observed below T_M . The splitting is due to the existence of two nonequivalent positions of the vanadium atoms in the tetragonal phase.⁶ We label these nonequivalent positions c (on chains parallel to the tetragonal C axis) and a (on chains) perpendicular to the C axis). The structure of the NMR spectra below T_M points to production of a system of domains whose tetragonal axes are distributed among the three principal axes of the crystal, and can be described as superposition of four spectra from the following configurations: $c, \theta = 0^\circ$; $c, 90^\circ$; $a, 0^\circ$, and $a, 90^\circ$. We observe no signs of the presence of a cubic phase below T_M .

In Table I are compared our data on the quadrupole-interaction constants in the tetragonal phase with the NAR data at 17 K.¹⁰ Although the differences $V_c - V_a$ are in reasonable agreement, the values are of V_c and V_a themselves differ substantially. Moreover, the results of Buttet and Lauger¹⁰ correspond to the inequality $V_{\text{cub}} < V_a < V_c$. At the same time a qualitative study of the possible change of the lattice and electric contributions to the EFG in the structural transition of V_3Si leads to the result $V_a < V_{\text{cub}} < V_c$, which agrees with our data as well with data for polycrystalline V_3Si .^{6,7} We note that a detailed comparison of our data below T_M with the results of Ref. 10 is difficult, inasmuch as in Ref. 10 they observed superposition of only three "uniaxial" spectra, which were ascribed to the configurations $c, 90^\circ$; $a, 0^\circ$, and $a, 90^\circ$. To explain this fact it was assumed that the tetragonal axes of all the domains lie in one plane (100), and the magnetic field was perpendicular to this plane. This assumption, however, was not verified for other orientations of H , so that one cannot exclude the possibility of ambiguous identification of the lines. If it is assumed that lines of the type $(a, 0^\circ)$ were not observed in Ref. 10 because of the insufficient signal/noise ratio, while the lines identified there as $(a, 0^\circ)$ pertain to the type $(c, 0^\circ)$, then the agreement between the results of Ref. 10 and our data becomes much better. An analysis of the cited data under this assumption leads, in particular, to the correct relation $V_a < V_{\text{cub}} < V_c$ and to a much lower value of the asymmetry parameter η_a .

Figure 2 shows the temperature dependence of the difference of the constants of the quadrupole interaction in the positions c and a . The growth of this quantity with decreasing temperature is due to the growth of the tetragonal deformation. It is therefore interesting to compare the behavior of $V_c - V_a$ with the temperature dependence of the lattice parameters in the tetragonal phase. Figure 2 shows also the temperature dependences of the lattice parameter C for two V_3Si single crystals with complete transformation.¹⁷ As seen from Fig. 2, the character of the temperature dependence of

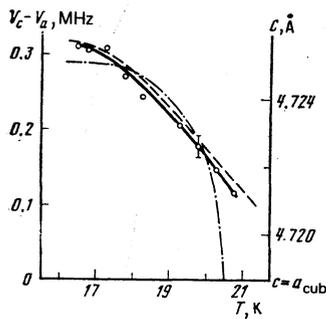


FIG. 2. Temperature dependence of the difference of the constants of the quadrupole interaction $V \equiv e^2 qQ/\hbar$ in positions c and a (experimental points, solid curve) and temperature dependence of the lattice parameter C as given by x-ray data¹⁷ in V_3Si : dash-dot curve—"typical" single crystal, $T_M = 20.5$ K; dashed curve—"untypical" single crystal that preserves tetragonality to 27 K.

$V_c - V_a$ in our sample recalls the behavior of the lattice parameter in a "nontypical" V_3Si single crystal, which preserves tetragonality up to 27 K.

4. Knight shift, spin-lattice relaxation, and electronic-state density

Figure 3 shows the temperature dependences of the isotropic and anisotropic components of the Knight shift in the temperature interval¹¹ 16.5–77 K. At room temperature we have $K_{iso} = 0.58 \pm 0.01\%$, $K_{ax} = -0.015 \pm 0.005\%$.

The values of K_{iso} and K_{ax} were determined from the NMR spectra with the aid of a relation (1); the values of K_{iso} were corrected with account taken of the demagnetizing field in the sample¹⁰ and of the skin effect.¹⁸ In the analysis of the Knight shift in the tetragonal phase we have assumed conservation of its axial symmetry. The data presented in Fig. 3 for $T < T_M$ pertain to positions of type a . The difference of the Knight shifts in positions a and c was within the limits of the experimental error.

At 77 K, the value of K_{ax} obtained by us agrees with the data of Refs. 8 and 10. At 17 K there is a discrepancy between our result and the value $K_{ax} = 0.07 \pm 0.01\%$ (for positions a) cited in Ref. 10. The possible cause of the discrepancy between our data and those of Ref. 10 at $T < T_M$ was discussed above.

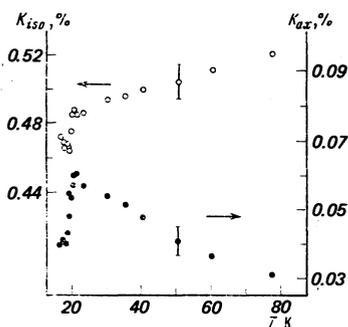


FIG. 3. Temperature dependence of the isotropic (light circles) and anisotropic (dark circles) components of the Knight shift of ^{51}V in V_3Si .

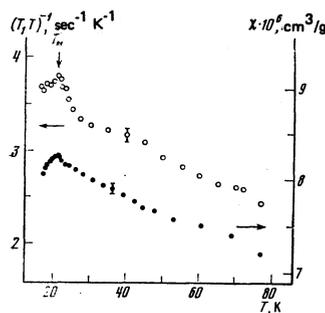


FIG. 4. Temperature dependence of the rate of spin-lattice relaxation (light circles) and of the magnetic susceptibility (dark circles) in V_3Si .

Figure 4 shows the temperature dependence of the rate of spin-lattice relaxation $(T_1 T)^{-1}$ together with the temperature dependence of the magnetic susceptibility in the interval 16.5–77 K. At room temperature,

$$(T_1 T)^{-1} = 1.43 \pm 0.07 \text{ sec}^{-1} K^{-1}, \quad \chi = (5.64 \pm 0.05) \cdot 10^{-6} \text{ cm}^3/g.$$

The strong temperature dependence of K_{iso} , K_{ax} , $(T_1 T)^{-1}$, and χ in the V_3Si can be attributed to the existence of a narrow peak of the electronic-state density near the Fermi level. The maxima of χ and of $(T_1 T)^{-1}$ are observed at the same temperature $T_M = 21.0$ K. Analogous maxima of χ at $T = T_M$ were observed earlier in V_3Si single crystals with $\alpha_R = 25$ and 34 .⁵ The decrease of $(T_1 T)^{-1}$ and χ below T_M is apparently connected with a decrease of $N(E_F)$ as a result of a structural transition. The behavior of K_{iso} and K_{ax} below T_M cannot be attributed only to the change of $N(E_F)$. In particular, the decrease of K_{iso} below T_M presupposes a substantial decrease of the orbital contribution to the Knight shift.

A joint analysis of the temperature dependences of K_{iso} , K_{ax} , $(T_1 T)^{-1}$, and χ in the cubic phase makes it possible to separate the contributions of different origin to these quantities and to determine certain details of the electronic structure of V_3Si . The quantity K_{iso} can be written in the form

$$K_{iso} = K^s + K_{iso}^{orb} + K^d(T) = \alpha \chi^s + \beta \chi_{iso}^{orb} + \epsilon \chi^d(T), \quad (2)$$

where the indices s , orb , and d denote respectively the contact contribution of the s electrons, the orbital contribution of the d electrons, and the spin contribution of the d electrons. The coefficients α , β , and ϵ are proportional to the corresponding hyperfine fields at the nucleus. The dependence of the experimental values of K_{iso} on χ in the cubic phase is well approximated by a straight line (Fig. 5) in accordance with (2). From the slope of this diagram we determine the hyperfine field of the polarization of the core: $H^d = -(0.70 \pm 0.08) \cdot 10^5$ Oe (per electron). The obtained value of H^d is noticeably lower in absolute magnitude than the value $H^d = -1.17 \cdot 10^5$ Oe for the V^{2+} ion, which is customarily assumed without any correction whatever also for metallic vanadium.¹⁹ This result is not unexpected if the strong covalence of the bonds in V_3Si is taken into account.

The standard procedure²⁰ for separating the contributions to K_{iso} and χ is in many cases not very reliable because the orbital hyperfine field H^{orb} is not

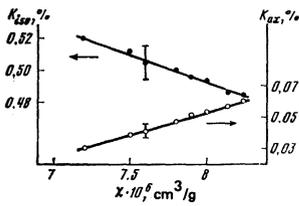


FIG. 5. Plots of K_{iso} (dark circles) and K_{ax} (light circles) against the magnetic susceptibility in V_3Si (the implicit parameter is the temperature).

known with sufficient accuracy. We have therefore used a method based on the reconciliation of the temperature dependences of $(T_1 T)^{-1}$ and χ , in which H^{orb} is determined by an iteration procedure. The method consists in the following. At a certain trial value of H^{orb} the contributions to K_{iso} and χ are separated by the known graphical method²⁰ based on the relation (2), and $\chi^d(T)$ is obtained. The obtained $\chi^d(T)$ yields the effective state density $N(T)$ of the d electrons on the Fermi level, from the equation

$$\chi^d(T) = 2\mu_B^2 N(T) / [1 - JN(T)],$$

where

$$N(T) = - \int N(E) \frac{\partial f}{\partial E} dE,$$

f is the Fermi function, $N(E)$ is the d -electron state density, μ_B is the Bohr magneton, and J is the exchange integral (an estimate by Clogston's method²¹ yields $J = 0.14$ eV). Neglecting the contribution of the s electrons to the relaxation rate, we can write²⁾

$$(T_1 T)^{-1} \sim N^2(T).$$

We require that the ratio $(T_1 T)^{-1} / N^2(T)$ remain constant in the entire investigated temperature interval. If this is not the case, then this procedure is repeated for other values of H^{orb} until the temperature dependences of $N^2(T)$ and $(T_1 T)^{-1}$ are reconciled. The best agreement in the temperature interval 24–293 K was reached at $H^{orb} = (1.85 \pm 0.05) \cdot 10^5$ Oe (per Bohr magneton). We note that the orbital hyperfine field in metallic vanadium was assumed to be 1.9×10^5 Oe.¹⁹ To estimate the small s -contribution to χ we have assumed $\chi^s = 0.2 \cdot 10^{-4}$ cm³/mole, and, using the value of the contact hyperfine field in metallic vanadium $H^s = 11.2 \cdot 10^5$ Oe,¹⁹ obtained $K^s = 0.07\%$. The results of separation of the d -electron contributions to χ and K_{iso} at 25 K are the following:

$$\begin{aligned} \chi_{iso}^{orb} &= 5.2 \cdot 10^{-4} \text{ cm}^3/\text{mole} \quad K_{iso}^{orb} = 0.59\%, \\ \chi^d &= 9.3 \cdot 10^{-4} \text{ cm}^3/\text{mole} \quad K^d = -0.17\%. \end{aligned}$$

The anisotropy of the Knight shift is due to the anisotropy of the dipole hyperfine field and the anisotropy of the orbital susceptibility:

$$K_{ax} = K_{ax}^{dip} + K_{ax}^{orb}.$$

The dipole contribution can be written in the form²²

$$\begin{aligned} K_{ax}^{dip} &= - \frac{1}{2} \int d\mathbf{r} \frac{B(\mathbf{r})}{r^3} P_2^0(\cos \rho), \\ B(\mathbf{r}) &= 4\mu_B^2 \sum_k \frac{\partial f}{\partial E_k} |\psi_k(\mathbf{r})|^2, \end{aligned}$$

where $\psi_k(\mathbf{r})$ are the eigenfunctions of the electron Hamiltonian $P_2^0(\cos \rho)$ is the associated Legendre polynomial, and ρ is the angle between \mathbf{r} and the symmetry axis. In the tight-binding approximation we obtain for the A-15 structure

$$K_{ax}^{dip}(T) = \frac{2}{3} \chi^d(T) \langle r^{-3} \rangle [F_\sigma + F_\pi - F_{\delta_1} - F_{\delta_2}], \quad (3)$$

where $\langle r \rangle$ is the average distance of the d electron from the nucleus (averaging over the radial part of the wave function), F_i are the relative weights of the wave functions of symmetry $\sigma(z^2)$, $\pi(xz, yz)$, $\delta_1(x^2 - y^2)$, and $\delta_2(xy)$ on the Fermi level,

$$F_\sigma + F_\pi + F_{\delta_1} + F_{\delta_2} = 1. \quad (4)$$

It is seen from (3) that the temperature dependence of K_{ax} imposes definite restrictions on the relation between the coefficients F_i and makes it possible therefore to select the possible types of the band structure, in particular, the dominant contribution to the δ states on the Fermi level (as in the Labbe-Friedel model²⁾ does not agree with the sign of the temperature dependence of K_{ax} . The dependence of the experimental values of K_{ax} on above T_M is well approximated by a straight line (Fig. 5). We can therefore assume that K_{ax}^{orb} does not depend on temperature, and the entire temperature dependence of K_{ax} is determined by the term K_{ax}^{dip} , which is proportional to $\chi^d(T)$. Using the obtained value $H^{orb} = 2\mu_B \langle r^{-3} \rangle = 1.85 \cdot 10^5$ Oe, we get from the slope of the plot of $K_{ax}(\chi)$

$$F_\sigma + F_\pi - F_{\delta_1} - F_{\delta_2} = 0.84. \quad (5)$$

We can now determine the contributions of K_{ax}^{dip} and K_{ax}^{orb} . At 23 K we have

$$K_{ax}^{dip} = 0.123\%, \quad K_{ax}^{orb} = -0.066\%.$$

To determine the coefficients F_i we use data on the spin-lattice relaxation. In the tight-binding approximation, without allowance for the contribution of the s electrons to the s - d mixing, we can write²³

$$(T_1 T)^{-1} = 2h\gamma^2 k_B N^2(T) [(H^d)^2 R_d + (H^{orb})^2 R_{orb}]. \quad (6)$$

Here k_B is the Boltzmann constant and R_d and R_{orb} are expressed in terms of the coefficients F_i and depend on the crystal symmetry; R_{orb} can also depend on the orientation of the magnetic field. For the A-15 structure at H \parallel [111] we have obtained

$$R_d = F_\sigma^2 + F_{\delta_1}^2 + F_{\delta_2}^2 + \frac{1}{2} F_\pi^2, \quad (7)$$

and

$$R_{orb} = \frac{1}{3} F_\pi (6F_\sigma + \frac{1}{2} F_\pi + 2F_{\delta_1} + 2F_{\delta_2}) + \frac{2}{3} F_{\delta_1} F_{\delta_2}. \quad (8)$$

Since F_{δ_1} and F_{δ_2} enter in Eqs. (3), (7), and (8) in like fashion, we cannot distinguish between them. We put $F_\delta = F_{\delta_1} + F_{\delta_2}$ and consider two extreme cases: a) one of the coefficients $F_{\delta_1}, F_{\delta_2}$ is equal to zero, b) $F_{\delta_1} = F_{\delta_2}$. Making the corresponding changes in (4) and (5), (7) and (8) and solving equations (4)–(8) simultaneously, we get F_σ, F_π , and F_δ .

The results of the separation of the contributions to the effective density of the electronic states on the Fermi level $N_f(T) = F_i N(T)$ and to the rate of the spin-lattice relaxation at 25 K for versions (a) and (b) are given in Table II. As seen from this table, the results

TABLE II.

Variant	N_G	N_π	N_δ	N	$(T_1 T)_{orb}^{-1}$	$(T_1 T)_d^{-1}$	$(T_1 T)^{-1}$
	(eV · spin) ⁻¹				(sec · K) ⁻¹		
a	0.23	2.40	0.23	2.86	2.93	0.52	3.45
b	0.22	2.41	0.23	2.86	2.95	0.50	3.45

depend very little on the relation between F_{δ_1} and F_{δ_2} . The dominant contribution to the state density on the Fermi level is made by the π symmetry states. This conclusion does not agree with the calculations of the band structure in V_3Si (Ref. 24), which predict that the main contribution to $N(E_F)$ is made by states of δ_1 symmetry. The latter, as already noted, contradicts the data on K_{ax} . In addition, the state density near the Fermi level should change substantially over an interval of the order of 10^{-2} eV, so as to ensure the observed temperature dependences of $(T_1 T)^{-1}$ and χ , and the energy resolution in the band calculations²⁴ is of the order of 10^{-1} eV. Thus, the resolution of the band calculations²⁴ is not high enough for a detailed comparison with the experimental data. We note also that in the preceding attempts to determine the coefficients F_i in A-15 compounds^{25,26} they used in (6) in place of $N(T)$ the state density $N(0)$ obtained from low-temperature measurement of the specific heat, and the value of $(T_1 T)^{-1}$ was taken at 77 K. In other words, no account was taken in Refs. 25 and 26 of the strong temperature dependence of the quantity $(T_1 T)^{-1}$.

It should be noted that in the case of a rigorous analysis Eq. (6) contains $N^2(T)$ in the form

$$\int N^2(E) \frac{\partial f}{\partial E} dE,$$

and not in the form

$$\left(\int N(E) \frac{\partial f}{\partial E} dE \right)^2,$$

which was in fact used by us. The error introduced on account of this approximation into $N^2(T)$ in the region of the low temperatures at which the measurements were made does not exceed 20%. The corresponding correction does not lead to a substantial change of the picture of the separation of the contribution.

We note in conclusion that the scheme proposed by us for the analysis of the experimental data makes it possible to establish the connection between the temperature dependences of K_{iso} , K_{ax} , $(T_1 T)^{-1}$ and χ in the cubic phase. This analysis necessitated, of course, a number of simplifying assumptions. We have assumed, in particular, that the d -wave functions of different symmetry have the same radial dependence, and this regarded the s - d hybridization. As shown above, the temperature dependences K_{ax} and AS impose definite limitations on the possible form of the band structure of V_3Si . Although the accuracy of the separation of the contributions to $N(T)$ is estimated by us at 20%, our re-

sult apparently reflect correctly the main features of the electronic structure on the Fermi level in V_3Si , which are directly connected with the experimentally measured NMR parameters.

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¹All figures show the maximal absolute errors in the determination of the measured quantities. The relative errors, on the other hand, which are important for the determination of the temperature dependences, are noticeably lower (in particular, by a factor of 3 in the case of K_{iso}).

²We do not take into account the influence of the electron-electron interaction on T_1 , since the dominant contribution to the relaxation rate is made by the orbital hyperfine interaction, which is not renormalized when exchange is taken into account.

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