[7] V. N. Tsytovich, Teoriya turbulentnoĭ plazmy (Theory of turbulent plasmas) Atomizdat, 1971 [translation to be published by Plenum Press].
[8] A. G. Litvak, G. M. Fraĭman, and A. D. Yunakovskiĭ, Pis'ma Zh. Eksp. Teor. Fiz. 19, 23 (1974) [JETP Lett. 19, 13 (1974)].

Translated by D. ter Haar

Nuclear magnetic resonance of V^{51} in a V_3Si single crystal at room temperature

B. N. Tret'yakov, V. A. Marchenko, and V. B. Kuritsin

Central Research Institute for Ferrous Metallurgy
(Submitted January 20, 1975)
Zh. Eksp. Teor. Fiz. 70, 1795–1797 (May 1976)

NMR of V^{51} in a V_3Si single crystal is investigated at room temperature. The anisotropic component K_{an} of the Knight shift is found to be zero. It is noted that calculations based on the band-structure scheme proposed by Labbe and Friedel are not in accord with the obtained temperature dependence of K_{an}.

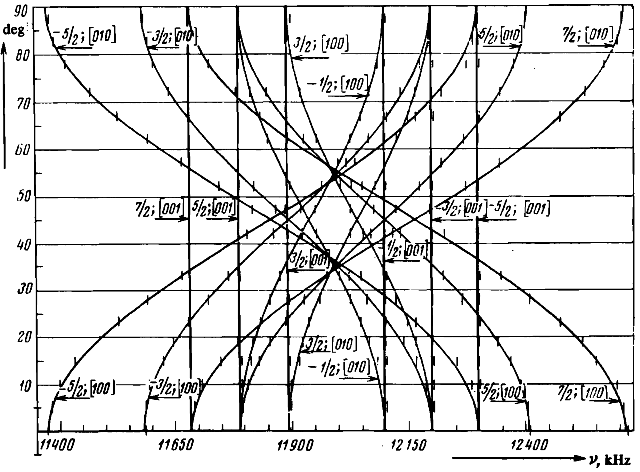
PACS numbers: 33.30.De, 76.60.Cq

Tret'yakov, Kodes, and Kuritsin,[1] in a report of the results of an investigation of nuclear magnetic resonance (NMR) of V^{51} in polycrystalline V_3Si samples, have shown that in addition to the temperature-dependent isotropic Knights shift (K_{is}) there exists an anisotropic component of the Knight shift (K_{an}), which also changes with changing temperature. Since there was no sufficiently correct method of determining K_{an} from the NMR spectra obtained with polycrystals until recently, it was impossible in[1] to determine K_{an}. However, since K_{an} is directly connected with the anisotropy of the electron density in crystals, and in some cases with the values of the magnetic moments of the atoms contained in the crystal lattice, attempts were made to investigate NMR in single-crystal samples of V_3Si. Tret'yakov *et al.*[2] investigated NMR of V^{51} of single-crystal V_3Si in a polarizing magnetic field $H_0 = 4$ kOe at 78 °K and have established that $K_{an} = 0.04\%$ for this resonance. The use of the acoustic nuclear resonance method,[3] likewise with a single-crystal sample, has confirmed the value $K_{an} = 0.04\%$ at 78 °K, and yielded $K_{an} = 0.07\%$ at 17 °K. At room temperature, however, the value of K_{an} for NMR of V^{51} has not been determined to date.

The present study is a continuation of[2] and is devoted to an investigation of NMR of V^{51} in the same V_3Si single crystal, for the purpose of obtaining the value of K_{an} at room temperature. The experiment itself as well as the reduction of the experimental data were the same in the present study as in[2], except for the value of the polarizing magnetic field H_0, which could be raised to 10 kOe, owing to the increase in the resistivity of the sample at the higher temperature; this led to an increase in the accuracy of K_{an}. The accuracy with which the crystallographic directions of the single crystal were set relative to the external magnetic field was 2°.

The figure shows a plot of the resonance frequencies of the satellite NMR transitions of V^{51} on the angle φ between the direction of H_0 and the crystallographic direction [100] of the single crystal. The [001] direction remained perpendicular to H_0 for all the spectra. The vertical strokes in the figure correspond to the experimental values of the resonant frequencies, while the solid lines were calculated theoretically at $K_{an} = 0$, $K_{is} = 0.54\%$, and a quadrupole splitting constant $\nu_q = 206$ kHz. The method of determining these parameters from the experimental values of the satellite transition frequencies is given in[2]. Thus, the reduction of experimental data leads to the following NMR parameters of V^{51} in V_3Si at room temperature: $\nu_Q = 206 \pm 1$ kHz, $K_{is} = (0.54 \pm 0.01)\%$, and $K_{an} = (0.00 \pm 0.01)\%$.

The parameters of NMR of V^{51} using the spectrum from a powder obtained by pulverizing a part of the investigated single crystal has yielded the parameters $\nu_Q = 206 \pm 1$ kHz, $K_{is} = (0.57 \pm 0.01)\%$, and $K_{an} = (0 \pm 0.01)\%$. These parameters are identical with the parameters of



Dependence of the resonant frequencies of the NMR satellite transitions of V^{51} of single-crystal V_3Si on the crystal orientation relative to the external magnetic field at room temperature. The fractions in the figure correspond to the quantum magnetic number of the Zeeman level of the V^{51} nucleus.

T, K	ν_Q, kHz	K_{is}, %	K_{an}, %
300	206±1	0.57±0.01	0.00±0.01
78	205±1	0.48±0.02	0.04±0.015

the NMR of V^{51} in the single-crystal sample, with the exception of K_{is}. The discrepancy in K_{is} is due to the fact that in the reduction of the spectra of the single crystal no account was taken of the additional demagnetizing field due to the shape of the sample, or of the distortion of the shape of the satellite transitions due to the admixture of the dispersion signal. Allowance for this factor results in a correction 0.03% and eliminates the aforementioned discrepancy. In[2] principal attention was paid to obtaining a reliable value of K_{an}, and the corrections in question were not taken into account in the determination of K_{is}. The values of the NMR parameters of V^{51} at 78 and 300 °K, with allowance for all the corrections, are summarized in the table.

Thus, an additional anomaly of the physical properties of V_3Si is the temperature dependence of the anisotropic Knight shift with zero or near-zero value at room temperature.

The most probable cause of the appearance of K_{an} may be the hyperfine field H_{dip} due to the dipole-dipole interaction of the magnetic moment of the nucleus with the magnetic moment of the electrons, [4] since the point symmetry of the vanadium atoms in V_3Si is lower than cubic ($\bar{4}2$ m). If the Z axis is directed along the chain of vanadium atoms, then we can write for H_{dip} [3]

$$\mathbf{H}_{dip} = -\left\langle \psi_d(k_F) \left| \frac{\mathbf{h}_0}{r^3} - \frac{3(\mathbf{r}\mathbf{h}_0)\mathbf{r}}{r^5} \right| \psi_d(k_F) \right\rangle \frac{\chi_d H_0}{6N},$$

where $\psi_d(k_F)$ is the wave function of the d electrons with Fermi energy, N is Avogadro's number, k_F is the wave vector of the d electrons on the Fermi surface, χ_d is the molar susceptibility of the d electrons, H_0 is the polarizing magnetic field, $\mathbf{h}_0$ is the unit vector directed along H_0, and $\mathbf{r}$ is the radius vector that determines the position of the d electrons relative to the considered nucleus. As seen from this expression, $K_{an}(T)$ should be proportional to $\chi_d(T)$.

According to Labbe's calculations[5] the temperature-dependence of the susceptibility $\chi_d(T)$ changes by a factor of seven in the temperature interval from 17 to 300 °K. At room temperature, within the framework of Labbe's model, $\chi_d(T)$ does not vanish (χ_d (300 °K) $= 1.1 \times 10^{-4}$ emu/mole). Taking these values into account together with the data of[3] (K_{an} (17 °K) = 0.07%) we can expect K_{an} at room temperature to be of the order of 0.01%, which agrees with the results of our investigations within the limits of measurement errors. However, allowance for the concrete band structure proposed by Labbe and Friedel, [6] by using actual wave functions of the d electrons, did not lead to agreement between the theoretical and experimental values of K_{an}. [3] In addition, the reduction of the spectra from the single crystal yields a small negative value of K_{an} ($K_{an} = -0.005\%$) at room temperature, although the value of the errors does not allow us to state that K_{an} becomes negative.

Thus, to explain the obtained temperature dependence of K_{an} it is necessary to make more precise the theoretical band structure of intermetallides of the type V_3Si.

[1] B. N. Tret'yakov, B. N. Kodess, and V. B. Kuritsin, Izv. Vyssh. Uchebn. Zaved. Fiz. 5, 141 (1974).

[2] B. N. Tret'yakov, V. A. Marchenko, V. B. Kuritsin, and B. N. Kodess, Zh. Eksp. Teor. Fiz. 65, 1551 (1973) [Sov. Phys. JETP 38, 772 (1974)].

[3] J. Buttet and K. Laugez, Phys. Rev. B9, 4643 (1974).

[4] B. Bleaney, transl. in: Sverkhtonkie vzaimodeistviya v tverdykh telakh (Hyperfine Interactions in Solids), E. A. Turov, ed., Mir, 1970.

[5] J. Labbe, Phys. Rev. 158, 647 (1967).

[6] J. Labbe and J. Friedel, J. Phys. (Paris) 27, 153, 303 (1966).

Translated by J. G. Adashko