"ANOMALOUS" MUONIUM IN SEMICONDUCTORS

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Introduction

The muon channel of the PNPI synchrocyclotron started to operate in 1976, and a wide program of investigations with beams of slow muons has been under way since that time. A few important problems of muonium physics have been solved in experiments in the PNPI muon channel. The conditions of formation of the "normal" (Mu) and "anomalous" (Mu^*) muonium and of the diamagnetic fraction in silicon monocrystals of n- and p-conductivity, and their interaction with a substance lattice were investigated in a wide range of temperatures. A comparison of main experimental data characterizing the Mu^* state and the hydrogen-containing Si-AA9 centre, found by the EPR method in silicon, was performed. It was shown that the Si-AA9 centre is similar to Mu^* and is a hydrogen analogue of Mu^*. A qualitative microscopic model of the muon and muonium interaction in the target substance was proposed, in which essential roles are played by overthermal processes of the muon and muonium interaction with the partially ionized monocrystal lattice. For the first time, an experimental study of parameters of the quadrupole muonium interaction in α-quartz monocrystals was carried out. Changing of the value and sign of the muonium quadrupole constant caused by fast muonium diffusion in the crystal lattice of a sample was observed. The investigation of muonium quadrupole oscillations in a substance opens up new opportunities in the muonium method. This method allows us to study non-uniform (non-homogeneous) electric fields inside crystals. A new direct and independent method of studying the muonium to antimuonium conversion ($M \to \bar{M}$), based on registration of high energy electrons from the decay of antimuonium muon with a wide aperture magnetic spectrometer, was proposed and realized. The joint PNPI–JINR experiment on measuring the probability of the conversion process $M \to \bar{M}$ was carried out in the "surface" muon beam of the JINR phasotron with the equipment developed and fabricated at High Energy Physics Division of PNPI.

The results of studying characteristic states of the muonium atom in semiconductors are discussed below, and the most important result is the determination of the "anomalous" muonium nature. The discussed investigations were performed by incorporated efforts of scientists from PNPI (Gatchina), ITEP (Moscow), JINR (Dubna), PTI (Alma-Ata), INP (Minsk).

"Anomalous" muonium

In 1973 two (and more than two in several cases) frequencies not connected with the "normal" muonium behaviour were found by Brewer when studying the precession frequencies of muonium atoms in silicon at low temperature (77 K). A careful investigation of "anomalous" precession frequencies was performed by Patterson et al. (1978). The authors showed that the "anomalous" frequencies at temperatures lower than 85 K were observed for n- and p-conductivity silicon samples for alloy impurity concentration from 10^{12} up to 10^{16} cm^{-3}. It was determined that three different muon-containing systems can exist in silicon simultaneously at low temperatures: the "normal" muonium (Mu), the "anomalous" muonium (Mu^*), and the diamagnetic fraction (μ). At high temperatures (at 295 K), only the diamagnetic fraction was observed. The most completely investigated by the authors was a silicon sample of

p-conductivity with the impurity concentration of $\sim 10^{13}$ cm^{-3} at $T = 30$ K. The values and the numbers of the observed "anomalous" frequencies, as it was shown, depend on the sample orientation. The authors managed to describe the observed effects with the axial-symmetric hyperfine interaction Hamiltonian:

$$\mathcal{H}^* = A_\perp(S_x I_x + S_y I_y) + A_{||} S_z I_z - g_e m_e S H - g_\mu m_\mu I H \tag{1}$$

with the parameters $A_\perp = 92.1 \pm 0.3$ MHz, $A_{||} = 17.1 \pm 0.3$ MHz; here z is the axis of the crystal symmetry (axis [111]).

In works of Belousov et al. (1978) analytical solutions for energy levels of the "anomalous" muonium were obtained for all possible cases, and the formulae for calculating the polarization *vs* time were given. There are, probably, several physical reasons of appearance of the "anomalous" frequencies of the muon precession in silicon. One of the reasons is that the muon can occupy two positions of equilibrium in the silicon crystal lattice. In one of them – in the octapore of the monocrystal – the muonium is surrounded by the nearest atoms with the hexagonal orientation, so that the spherical symmetry of the hyperfine interaction is disturbed. Another scheme [1] is based on an assumption that there exists a muonium paramagnetic chemical bond with the silicon lattice. The experimental basis in favour of this or another display mode of three muon states in silicon can be obtained by studying the dependence of each state population on the temperature since, as an experience shows, in such a way it is possible to investigate characteristics of transitions between different states.

Molecular radical model for "anomalous" muonium

With the purpose of studying the mechanism of the muonium atom interaction in monocrystals of atomic semiconductors, systematic investigations of poor alloyed silicon samples of different conductivity were performed in the muon channel of the PNPI synchrocyclotron in a wide range of temperatures from 60 K to 730 K [1,2]. In experiments, the amplitudes of each of the three muon states in silicon at different temperatures, the relaxation speed of the mentioned states and possible transitions between them were determined. The experiments were performed both in the transverse and in the longitudinal magnetic fields. Under the condition of fast relaxation of the muon spin system, such an experimental method is more informative because a longitudinal magnetic field prevents significantly the influence of depolarizing factors.

Two silicon samples, one of the p-conductivity type with the concentration of admixture atoms of $\sim 5 \cdot 10^{12}$ cm^{-3}, and another of the n-conductivity type with the concentration of conductivity electrons of $1.6 \cdot 10^{13}$ cm^{-3}, were investigated in detail. Targets were made of identically oriented monocrystals whose conductivities and Hall constants had been measured previously.

A detailed description and an analysis of the experimental data are presented in Ref. [3]. We shall formulate here only basic facts following from the investigation performed.

1. The fraction of Mu component β(Mu) depends poorly on the temperature in both samples: β(Mu)=const in the temperature range 78 K $< T <$ 400 K. The amplitude of Mu component was calculated from the measured values of polarization in experiments with the longitudinal magnetic field of $H = 200$ Oe ($P = 0.73 \pm 0.02$ for p-silicon and $P = 0.67 \pm 0.03$ for n-silicon) using the known theoretical formulae in the assumption that the speed of the spin-exchange (frequency ν) and the chemical (characteristic muon stage time τ) interactions are small in comparison with the frequency of the hyperfine interaction ω: $\nu \ll \omega$ and $\omega\tau \gg 1$. The results are as follows: β(Mu)=0.56±0.05 and β(Mu)=0.69±0.06 for p- and n-silicon, accordingly.

2. The character of "restoration" of the muon polarization in the Mu^* state by the longitudinal magnetic field agrees with the conclusions of the theory. The experiment testifies that the Mu^* state exists in the temperature interval 78–204 K and at higher temperatures passes to the μ state. The fraction of Mu^* component $\beta(\mathrm{Mu}^*) = 0.39 \pm 0.03$ was calculated in agreement with the experimental data obtained with p-silicon at the temperature of 78 K (in conditions when precession frequencies of the Mu^* state were observed in the experiment).

3. The muon component of polarization at low temperatures is absent actually in n-silicon, while in p-silicon its fraction is $\beta(\mu)$=0.11$\pm$0.03. In the range of temperatures 300–400 K the fractions of the muon component are $\beta(\mu) = 0.50 \pm 0.02$ and $\beta(\mu)$=0.42$\pm$0.03 for p- and n-silicon, accordingly. These values, being compared with the indicated above values of $\beta(\mathrm{Mu})$, testify that the μ state has arisen from the Mu^* state.

4. In the range of temperatures $T > 400$ K, the speed of polarization relaxation grows sharply with the increase of temperature in both silicon samples in the transverse as well as in the longitudinal magnetic fields. It testifies that at $T > 400$ K the muon components stability is violated. A comparison of speeds of the polarization relaxation in the longitudinal and transverse fields (the longitudinal field does not prevent the relaxation, it reduces only its speed by a factor of 1.5–3) shows that products of the muon component decay are necessarily muonium atoms, and both the consecutive chain of transitions $\mu \Rightarrow \mathrm{Mu} \Rightarrow \mu \Rightarrow \ldots$ and the spin-exchange interactions of the muonium electron with the electrons of conductivity take place. On the basis of these facts a model of the chemical bond was proposed [1], according to which the muon interaction with the silicon may be described by the following schemes:

a) $\mu^+ + e^-$ (from the valency zone) $\Rightarrow \mathrm{Mu}$;

b) $\mathrm{Mu} + [\mathrm{Si}^+e^-e^-\mathrm{Si}^+] \Rightarrow [\mu^+e^-e^-\mathrm{Si}^+]\,\mathrm{Si}^+ + e^-$ (from the zone of conductivity);

c) $[\mu^+e^-e^-\mathrm{Si}^+]\,\mathrm{Si}^+ + e^-$ (from the zone of conductivity) $\Rightarrow [\mu^+e^-e^-\mathrm{Si}^+](\mathrm{Si}^+e^-)$.

The process a) is the muonium formation, and it is possible if the muonium ionization potential exceeds the width of the forbidden zone of the semiconductor. The process b) is interpreted as the transition $\mathrm{Mu} \Rightarrow \mu$, the activation barrier in silicon being equal to 0.18 eV. The process c) corresponds to the transitions $\mu \Leftrightarrow \mathrm{Mu}^*$. Here symbol Mu^* means the radical system $[\mu^+e^-e^-\mathrm{Si}^+](\mathrm{Si}^+e^-)$ in which the electron is located in one of the neighbour silicon atoms.

With the purpose of checking the model of molecular radical for the Mu^* state, we have studied how radiation defects influenced the ratio of amplitudes of the "normal" and "anomalous" muonium and of the diamagnetic fraction [4].

It is known that atoms of hydrogen in silicon interact actively with radiation defects of the lattice with the formation of a Si-H–type bond. A free muonium atom in silicon is an analogue of a hydrogen atom; the muonium finds quickly a dot defect and interacts with it, similarly to the hydrogen atom. As to the "anomalous" muonium behaviour dependence from the number of radiation defects in a sample, it is subject in many respects to the influence of the structure of this state. If we consider Mu^* to be a free muonium atom distinguished from Mu only by the hyperfine structure, the conditions of interaction of this system with the sample radiation defects should not differ significantly from the interaction of the Mu atom. If the Mu^* system is considered to be a complex rigidly fixed in the crystal lattice, then, on the contrary, the radiation defects cannot change dynamics of the Mu^* system behaviour in silicon because of the absence of diffusion in the sample.

For clearing up this question, the silicon sample of the p-conductivity type investigated by us earlier was exposed in a reactor to the radiation of fast neutrons. Initially, three series of irradiation by different doses of neutrons have been performed; they created, by estimations, the concentration of defects (displaced atoms) equal to: $2 \cdot 10^{18}$, 10^{17} and 10^{16} cm^{-3}. After each irradiation, μSR-measurements were performed with the irradiated sample and also with the same sample after the complete radiation defect annealing [4]. It is shown that:

1. The initial (at $t = 0$) polarization of muons both in the transverse and in the longitudinal magnetic fields does not depend on the defect concentration in the sample. It means that the radiation defects do not change the formation probability of the three states Mu, Mu* and μ.

2. Radiation defects influence in different way the "normal" and "anomalous" muonium in silicon (at $T > 0$). For the concentration of radiation defects within limits of 10^{16}–$2 \cdot 10^{18}$ cm^{-3}, the "normal" muonium is not observed experimentally: the precession at the muon frequency is not seen in the experiment. At the same time, the amplitude and the speed of the muon polarization relaxation in the "anomalous" muonium structure have not been practically changed. This fact testifies essentially different mobilities of the "normal" and "anomalous" muonium in the silicon crystal lattice. A subsequent annealing of the sample results in the restoration of the initial speed of the muon polarization relaxation in the "normal" muonium structure.

Further investigations carried out with the same silicon sample have shown [3] that the Mu precession frequencies are not observed even for the concentration of defects about 10^{13} cm^{-3}. A subsequent step-by-step isochronous annealing of the sample results in appearance of the relaxing Mu, the speed of relaxation exponentially falling with the increase of the annealing time. After the complete annealing, μSR-parameters of Mu are restored. The parameters of the Mu* state still remain constant.

Thus, we conclude from the experiments carried out at PNPI that the mobilities of the Mu and Mu* states in the sample are different. The Mu state diffuses quickly inside the lattice, while the Mu* state represents the object bound rigidly with the lattice of the sample, and it is in agreement with the mentioned above molecular radical model for the description of the Mu* state.

With the purpose of checking the universality of the mechanism of the muon and muonium interaction in a substance, a study of more complex semiconductors was accomplished [5,6]. For the first time, the existence of the Mu and Mu* states in the binary semiconductor GaAs was shown. The investigations were performed with a semi-insulating monocrystal sample of arsenic gallium alloyed with chrome ($\rho > 10^8\,\Omega\cdot$ cm, $[p] = 2 \cdot 10^{12}$ cm^{-3} at $T = 500$ K with the energy of activation of 0.69 eV) in the temperature range of 60–560 K. Temperature dependences of the initial amplitude and of the speed of the muon polarization relaxation were investigated in the transverse and longitudinal magnetic fields.

It is shown that the character of the dependence of the muon component of the polarization on the temperature in GaAs permits to select four temperature regions with various values of the initial polarization P [6]: I. 60–160 K – the polarization is constant and equal to $P = 0.12 \pm 0.02$; II. 160–200 K – a sharp increase of P up to the value of $P = 0.30 \pm 0.02$; III. 200–300 K – the monotonous decrease of P down to the value of $P = 0.20 \pm 0.02$; IV. 300–500 K – $P \simeq 0.2$; V. ($T > 500$ K) – a sharp increase of the initial polarization and the speed of muonium precession relaxation. The analysis of these data in comparison with the similar results for silicon permits to assume that the specific growth of the muon component of the polarization in the regions II and V is connected with the transitions between the states: Mu$^* \Rightarrow \mu$ (II) and Mu $\Rightarrow \mu$ (V). The absence of a plateau in the temperature dependence of the initial polarization in region III is connected, apparently, with the fact that the formed μ state in binary semiconductors is not stable.

Experiments with GaAs sample in longitudinal fields, being compared with the similar data for the silicon, demonstrate that the "anomalous" muonium exists in GaAs at $T < 170$ K and has a stronger hyperfine interaction (factor of strengthening is ~ 2–3).

A direct measurement of hyperfine splitting frequencies of Mu^* levels in monocrystals GaAs and GaP was carried out by Schneider et al. (1986). A comparison of the data for GaAs, GaP with the similar data for Si and Ge point to the universality of the mechanism of the muon interaction in crystal lattices of atomic and binary semiconductors.

Comparative analysis of properties of "anomalous" muonium and "anomalous" hydrogen

In the work of Gorelkinskii and Nevinnyi (1987) the paramagnetic state with the allowed hyperfine structure, resulting from hydrogen nuclei (Si-AA9 centre) implanted into a silicon sample at $T = 80$ K, was found out for the first time by the EPR method. The EPR-measurements in the absorption mode were performed with silicon samples after the implantation of hydrogen. For the implantation of hydrogen, the samples were irradiated by protons with the energy of 7 MeV through an aluminum absorber, the radiation dose being $5 \cdot 10^{14}$–$5 \cdot 10^{15}$ p/cm^2. The high purity samples of p-type silicon (ρ=6 kΩ·cm) and samples of p- and n-types (ρ=10 Ω·cm, thickness $\sim 300\,\mu$m) were investigated. The samples were illuminated with a tungsten lamp through a lightguide and a silicon IR-filter. The Si-AA9 centre was observed only for the illuminated samples ($W \sim 0.2$–0.3 W/cm^2). The Si-AA9 centre is a stable formation in a silicon lattice, it is always observed during a long time after the implantation of hydrogen, provided the samples are stored at temperatures lower than 180 K. The accomplished isochronous annealing of the samples shows [7] that in the temperature range of 190–210 K a relative fraction of the Si-AA9 centres decreases and at $T > 210$ K it irreversibly disappears. This is connected, apparently, with the annihilation of the paramagnetic configuration (by diffusion of hydrogen with the formation of a hydrogen molecule or a stable Si-H compound). In Ref. [7], a comparative analysis of experimental data on the formation of Mu^* and Si-AA9 is carried out. It is shown that the character of symmetry of the hyperfine interaction is identical for Mu^* and Si-AA9. Besides, the main values of the hyperfine interaction constants of the Si-AA9 centre correspond to the expected values of such constants for the "anomalous" hydrogen H^* (they are obtained by dividing the experimental values for Mu^* by the ratio $A_{\rm Mu}/A_{\rm H} = 3.14$ and are equal to: $A_\perp = \pm 29.3$ MHz; $A_{||} = \pm 5.4$ MHz). Experimental values of the constants of the superhyperfine interaction between ^{29}Si nucleus and electrons of Mu^* and Si-AA9 coincide practically. These values for Mu^* in Si (Si-AA9 in Si) are as follows:

$A_\perp(^{29}\text{Si}) = -73.96\,(72.9)$ MHz; $A_{||}(^{29}\text{Si}) = -137.5\,(128.9)$ MHz.

The temperature regions, in which the transition $Mu^* \Rightarrow \mu$ and the annihilation of the Si-AA9 centre occur, coincide also. Thus, the properties of the Si-AA9 centre are similar to the "anomalous" muonium properties. It allows to assert that the discussed centres have equivalent structures in silicon crystal, the difference being only in the presence of a muon in Mu^* instead of a proton in the case of Si-AA9 .

There exist several physical models for Mu^* in the crystal lattice of a semiconductor. One of the first models proposed was a model in which Mu^* was considered as the muonium located in a "hexagonal" point between nodes (Mu at point H, Fig. 1) of the crystal (Belousov et al., 1978). In another model [1], the muonium Mu^* was represented as a paramagnetic complex formed in a sample lattice as a result of the chemical interaction of the muonium atom with

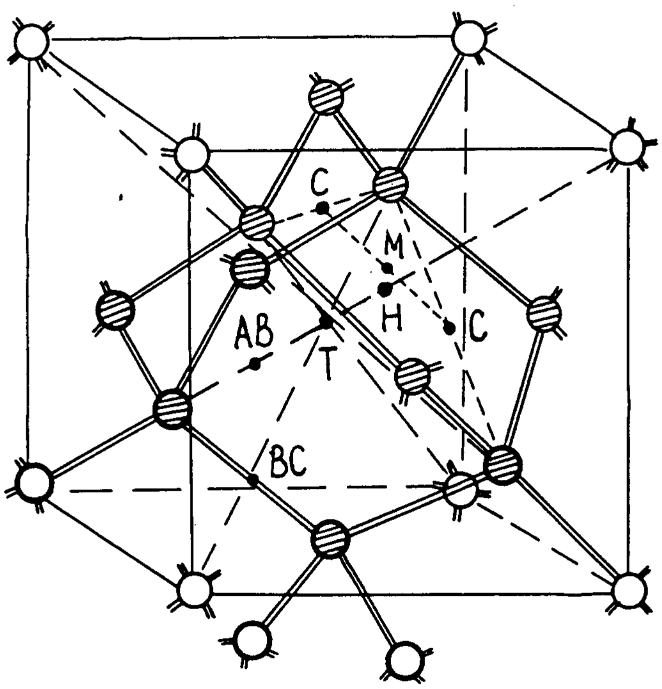

Fig. 1. Element of the silicon crystal lattice. Open circles – silicon atoms of cluster Si_8H_{16}, shaded circles – silicon atoms of cluster $Si_{10}H_{16}$. Points C, M, H, T, AB, BC – possible places of internode hydrogen.

atoms of the crystal lattice. In the frame of the model of complex Mu* with the localization of Mu in the middle of the bond between neighbour atoms of the crystal (point BC, Fig. 1) it was possible to explain some features of the parameters of the hyperfine interaction of Mu* in silicon and diamond (Cox and Symons, 1986). Similar results were obtained by Estreicher (1987) by considering Mu* as a vacancy complex. In our opinion, however, it seems improbable to bind the Mu* state with complex vacancies in the sample since, for example, the muon in the process of the thermolysis creates a small number of radiation defects (the main part of the muon energy goes to the ionization losses). Besides, the Mu* complex is formed with the probability of $\sim$ 40% in superpure samples of silicon. At last, as it is shown in Ref. [4], the injection of radiation defects to the sample up to the concentration of 10^{18} cm^{-3} does not increase the probability of the Mu* state formation. After the analysis of channeling experiments (channeling of muons from $\pi \rightarrow \mu$ decays and positrons from $\mu \rightarrow e$ decays in a crystal sample) Patterson (1984) assumed that Mu in Mu* is located at axis [111] in the contra-binding site (point AB, Fig. 1). Thus, we have several options for the site of the Mu atom in the Mu* complex.

With the purpose of obtaining new data on the possibility for the hydrogen-like atoms to be localized in semiconductors, the electronic structure of Mu, which is placed at points H, AB and BC of the crystal matrix of Si and diamond (C), was studied by us with the help of quantum-chemical methods. The program "spin-Hamiltonian" was used in our calculations. It allowed us to calculate not only the hyperfine interaction tensor, but also the electron g-tensor of the admixture atom. The calculations of the hyperfine interaction constant and the g-tensor were performed in the equilibrium geometry of the clusters simulating the Mu states in the lattice. For Mu at points H and AB, the clusters $MuX_{10}H_{16}$ (X=Si, C) centred at the tetrahedron point between the nodes (point T, Fig. 1) were calculated, whereas for Mu at point BC – the clusters MuX_8H_{18} with the centre at this point. The results of these investigations are given in detail in Refs. [8,9]. It is shown that the calculated properties of Mu at point BC are in qualitative agreement with the experimental characteristics of Mu^*. This means that Mu (H), located at lattice point BC, corresponds to the "anomalous" muonium (hydrogen) description. At the same time, it is not possible to exclude a dynamic model of the complex, according to which the muonium atom (the hydrogen) displaced from the bond axis X-X rotates (or tunnels) quickly around this axis. The validity of this representation was confirmed by the results of the experimental study of the superhyperfine interaction of the paramagnetic complex with the ^{29}Si nucleus for Si-AA9 (Gorelkinskii and Nevinnyi, 1987) and Mu^* (Kiefl et al., 1988). It was shown that the structure of the centre Si-AA9 (H^*) and Mu^* includes two equivalent silicon atoms located along axis [111] at identical distances from the hydrogen nucleus and the muon.

The analysis of the electronic structure of complexes simulating the muonium atom (hydrogen) at points BC of the silicon and diamond crystals shows that in all cases there is a donor level inside the forbidden zone. This fact permits evidently to explain the necessity of the sample illumination for detecting the "anomalous" hydrogen (Si-AA9) in silicon. Indeed, the "anomalous" hydrogen (H at point BC), being a donor, gives back an electron to acceptors, and its level (paramagnetic) becomes empty (diamagnetic). To fill it, an illumination which delivers electrons from the valency zone to this empty level, is necessary. Admixture atoms, as well as structural defects, injected during the low temperature implantation process can play the role of possible acceptors in Si.

It is necessary to note that a weak isotopic dependence of the constants of the hyperfine and the superhyperfine interactions exists for the "anomalous" muonium and hydrogen. To understand the nature of this isotopic dependence, it would be important to investigate the "anomalous" deuterium D^* and tritium T^* in detail. In our opinion, the study of isotopic effects in the region of low (< 10 K) temperatures will allow us to find out whether the static or dynamic version of the model of the "anomalous" hydrogen-like centres takes place in semiconductors.

The experimental detection of the centre Si-AA9 – a hydrogen analogue of the "anomalous" muonium – permits us to reanalyze the rich μSR-information obtained in the last 20 years in studies of the muonium characteristic states in semiconductors. Indeed, it was considered until recently that these states were unique only for the muon interaction in semiconductors. The data presented above show common features in interactions of muonium, hydrogen and other hydrogen-like systems in the crystal structure.

A picture of muon and muonium interaction in substance

In works of Cox and Symons (1986) and of Estle et al. (1986) an attempt to generalize the existing experimental material and to construct a realistic model for muon interaction in the substance is done. The model of the description of Mu^* as a molecular radical, which was considered for the first time in our work [1], is becoming generally accepted now. In the majority of cases the offered models of the muon interaction are supported by results of quantum-mechanical calculations. However, these models explain only some properties of the "anomalous" muonium, and do not give the solution of the general problem. In particular, the experimental fact (see Sect. 3) that the Mu^* properties are not connected with the defects injected to the sample by a radiation has not been explained.

A qualitative microscopic model of the muon interaction with the target substance from the moment of the thermolysis till the moment of the muon decay is given below. In the model under consideration, an essential role is played by overthermal processes occurring in time intervals smaller than 10^{-10} s, during which the formation of all observable states (including muon) and their thermolysis occurs. An important part of the present consideration is the interaction of the muon with its track for times from $\sim 10^{-12}$ s up to the complete muon stop.

We shall divide conditionally the time scale of the muon interaction in a substance to four intervals relative to the time $t = 0$ – the moment of the muon complete stop: I. from -10^{-10} to -10^{-12} s, II. from -10^{-12} to $5 \cdot 10^{-11}$ s, III. from $5 \cdot 10^{-11}$ to $5 \cdot 10^{-9}$ s, IV. from $5 \cdot 10^{-9}$ to 10^{-5} s (I – the interval of "negative" time connected with the muon track formation and thermolysis processes; II – the interval of the "hot-chemistry channel" when the muon polarization is not lost; III – the interval of the fast muonium depolarization owing to the hyperfine interaction and processes of spin-spin exchanging of the Mu electron with the environment electrons; IV – the interval of the slow muon depolarization). Only the states of the muon polarization in the time interval IV are accessible for measurements in an experiment, they depend essentially on processes occurring in the intervals I – III.

The behaviour of muons in the interval I is determined mainly by losses of a significant energy (~ 30 keV) in this time interval inside a small volume with linear size of $\sim 10^{-6}$ m during the thermolysis process, which results in appearance of electron defects like bond breaks. These defects facilitate formation of a stable complex inside the molecular lattice of the crystal by the process of the multiple muon charge exchange $\mu^+ \Leftrightarrow$ Mu . The further behaviour of the muon spin in the complex structure depends strongly on the charge state of the complex, the bond mode, the activation energy, and the spins of the adjacent atoms. Just in the interval I the initial formation of characteristic states containing muon occurs. The Mu* states and the fraction of μ states bound with the diamagnetic complex are fixed at certain nodes of the crystal lattice (we remind that Mu is the free muonium atom, Mu* is the paramagnetic molecular complex, μ is the diamagnetic molecular complex or a free muon). The Mu atoms are fixed at positions between the nodes only for low enough temperatures (lower 40–120 K depending on the structure of the target substance). At high temperatures they diffuse freely inside places between the nodes of the lattice. The diffusion of the free muon depends strongly on the sample purity and is investigated in detail for a large number of target materials. The muon polarization in all initial states coincides with the polarization of the muon beam.

The time interval II is essential for the Mu state and for the free muon in the range of temperatures, in which diffusion speeds of Mu and the muon inside a crystal are rather high, and is responsible for possible transitions between the states Mu $\Leftrightarrow$ Mu*, Mu $\Leftrightarrow \mu$, $\mu \Leftrightarrow$ Mu*. The transitions in Mu* depend mainly on the structure of the conductivity and valency zones of the target substance. The latter depends, in turn, on the sample temperature and on the number of residual electron defects during track dissipation. Thus, the state of the muon polarization is not changed.

The time interval III is characterized by the existence of the muon depolarization process in the Mu atom due to the hyperfine interaction in the state with $m = 0$ (m – magnetic quantum number) and in Mu* due to the hyperfine and superhyperfine interactions (if nuclei with non-zero spin are available in the molecular lattice structure). The degree of muon depolarization depends strongly on the character of the conductivity zone and on the structure of defects in a sample and can vary from $P/2$ to 0 (P – the initial polarization of the μ^+ beam).

Thus, the initial polarization of muons in different states measured experimentally depends on the processes occurring in time intervals I – III. Further development in time (the interval

IV) depends essentially on the availability of internal magnetic and non-uniform electric fields, their orientation relatively to the crystal symmetry axes and is well investigated now for the majority of samples containing the long-lived muonium.

Calculations of equilibrium configurations of hydrogen in silicon were performed by us to check the energy stability of paramagnetic complexes in the monocrystal lattice with hydrogen (muonium) placed at the broken bond [10]. The self-consistent discrete-variational X_α-method

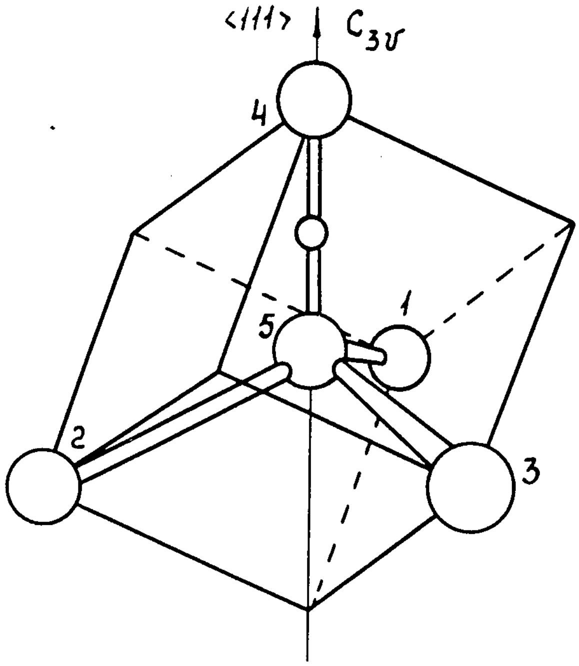

Fig.2. Element of Si_5H_{12} cluster of silicon crystal lattice . 1, 2, 3, 4, 5 – Si atoms.

(DVM-X_α), developed for numerical integrations of one-electron Hartree–Fock–Slatter levels, was used for the calculations. The one-electron Hamiltonian H of the system included the following operators: Δ – kinetic energy, V_n — interaction of electrons with nuclei of the system; V_c – the Coulomb interaction of electrons and nuclei, V_{X_α} – local exchange potential:

$H = -\frac{1}{2}\Delta + V_n + V_c + V_{X_\alpha}$.

The calculations were performed with the original version of the program DVM-X_α (Gutsev and Miakenkaia, 1988) using numerical Hartree–Fock functions of the ground states of Si and H atoms. The Si_5H_{12} cluster simulating a fragment of the silicon lattice had the structure of diamond with the bond length $d = 2.35$ Å. Being implanted into such an ideal cluster Si_5H_{12}, the hydrogen atom was placed at the broken bond in the centre of Si-Si (Fig. 2). The symmetry of the defect in this case is C_{3v}, and the axis of symmetry is [111]. The dependence of the total energy on the value of the displacement of the centred hydrogen is shown in Fig. 3. It is seen that in the middle of the bond the hydrogen occupies a stable position relative to the displacement along the bond line, which agrees with the data presented above for the Si-AA9 centre.

Another situation arises in the lattice in the case of excitation and ionization of two and more bonds between silicon atoms. Such an excitation leads to the displacement of the silicon atom into the place between the nodes. The similar mechanism of vacancy formation at

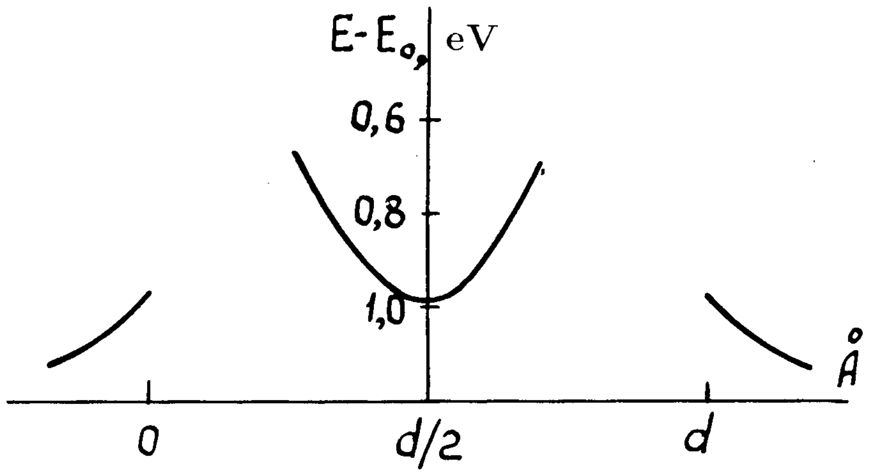

Fig.3. Total energy of $SiHSi_4H_{12}$ cluster as a function of the hydrogen displacement from the equilibrium position ($d/2$) in the bind-centred configuration, and the same for Si atoms (4 and 5) at the synchronous displacement to different sites (d = 2.35 Å).

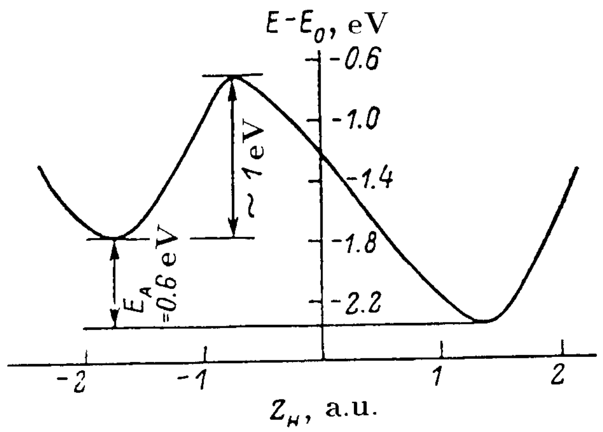

Fig.4. Total energy of H + □ Si_4H_{12} cluster for variations of H positions.

subthreshold energies in semiconductors is confirmed by several independent methods of the registration of radiation effects: by the method of radioactive isotopes, by the measurement of voltage-capacitance, voltage-current and spectral characteristics of the diode structures, by the measurement of the conductivity and mobility. The evaluation of the cross section for defects formation due to the ionization caused by the subthreshold radiation gives a value of the order of 1 b for germanium, that is comparable with the cross section for defects creation for the overthreshold radiation. The energy to create such a vacancy in the silicon is 2–4 eV.

It is natural that the arisen vacancy captures the hydrogen atom. The behaviour of the hydrogen atom was simulated with the use of the Si_5H_{12} cluster from which the central silicon atom was removed and the hydrogen atom was placed at one of the broken bonds of the neutral vacancy (p) in the [111] direction [10]. The C_{3v} symmetry of the system remained the same. The spin-limited version of the program DVM-X_α was used for the calculations. Two minima in the curve (Fig. 4) of the total energy as a function of the H atom displacement correspond to stable configurations of hydrogen in the H + □ Si_4H_{12} cluster.

It is easy to see that the discussion presented here is connected with one of possible mechanisms of the vacancy model. However, the probability of such a process is small, and it cannot be treated as the main one when considering "anomalous" muonium models. It is necessary to note also that the discussed above calculations for the vacancy $\square\, Si_4H_{12}$ should be considered only as an estimate, because to employ the vacancy model for calculations it is not sufficient to take into consideration only the cluster Si_5H_{12}. One needs to take also into account the silicon adjacent atoms of the monocrystal.

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4. APPLIED INVESTIGATIONS