EQUIVALENT STATES OF MUONIUM AND IMPLANTED HYDROGEN IN SILICON

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Experimental studies of the HFL of muon and electron magnetic momenta in a μ^+e^- atom implanted into a silicon crystal reveals the presence of two bound states which have been named «normal» (Mu) and «anomalous» (Mu*) muonium. Mu is an isotropic system. Mu* is an anisotropic but axially symmetric system. Systematic studies have been made /1,2/ on the conditions of formation and on the dynamics of interaction between the Mu, Mu* and μ^+ states (μ^+ is a diamagnetic compound of a Mu atom and lattice atoms, i. e. type Si-H compound) in n- and, p-silicon. Temperature ranges have been found where dynamic transitions between these states occur. A scheme is suggested for the muon interaction in silicon where the Mu* symbol specifies this type of molecular radical $[i^+e^-e^-\mu^+](Si^+e^-)$.

Table

Principal values of the g-AND A-tensors of AA9 and Mu* centers.
$A_\parallel \parallel [111]$; $g_1 \parallel [111]$

Center	g-factor	A (^{1}H)	A (^{29}Si)
Si—AA9	$g_1=2{,}0011\,(3)$ $g_2=1.9983\,(3)$ $g_3=1.9983\,(3)$	$A_\parallel=6.2\,(1.0)$ $A_\perp=31.4\,(1.0)$	$A_\parallel=128.9\,(1.0)$ $A_\perp=72.9\,(1.0)$
Mu*	$g=2$	$A_\parallel=5.53\,(1)$ [a] $A_\perp=29.46\,(1)$ [a]	$A_\parallel=137.5\,(1)$ [b] $A_\perp=73.96\,(5)$ [b]

a) Taken from /6/ and scaled by the ratio of muon and proton magnetic momenta (3.1423).
b) Taken from /7/.

Despite a wealth of experimental data on Mu and Mu*, the nature of these centers has not been fully clarified. Until recently, the situation was considerably aggravated by the fact that no one has observed hydrogen (H) — bearing analogues of Mu* centers in semiconductors. These difficulties have been partially overcome by now thanks to a recent discovery of a new paramagnetic center Si—AA9 in silicon by ESR /3/. Gorelkinskii et al /3/ studied ESR spectra following the implantation of hydrogen into silicon at T=80 K. To produce implantation, silicon samples were irradiated by 7 MeV/nucl. protons or deuterons.

A comparative analysis of the μSR and ESR experimental data shows that the parameter of the Si—AA9 center agree remarkably with those of the Mu* state /4/. The exact axial symmetry with respect to the [111] Si axis of the HFI for Mu* and Si—AA9 and the coincidence (taking into account the isotope effect) of the HFI constants (table) and of the temperature regions of stability for Si—AA9 and Mu* (fig. 1) suggest the existence in silicon of two equivalent structures, Mu* and Si—AA9, differing only in the mass of the hydrogen center.

During the last two years we have been studying the electronic structure of Mu(H) located at the hexagonal (H) and the bond-centered (BC) interstitial sites of Si and C crystals using the well-known semiempirical INDO method /5/. We focus our attention on the calculation of the HFI tensors and the electronic g-tensors of the impurity atom at the considered sites. The calculations of the above tensors were performed in the equilibrium geometry of the finite clusters, modelling Mu states in a crystal. The calculations of properties of clus-

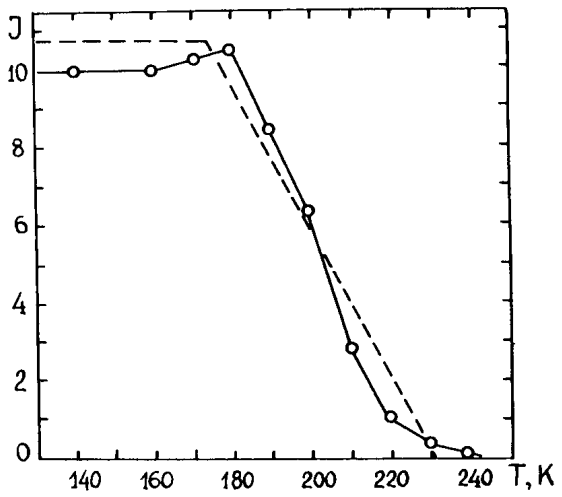

Fig. 1. Temperature range of stability for Si—AA9 (solid curve) and Mu* (dashed line)

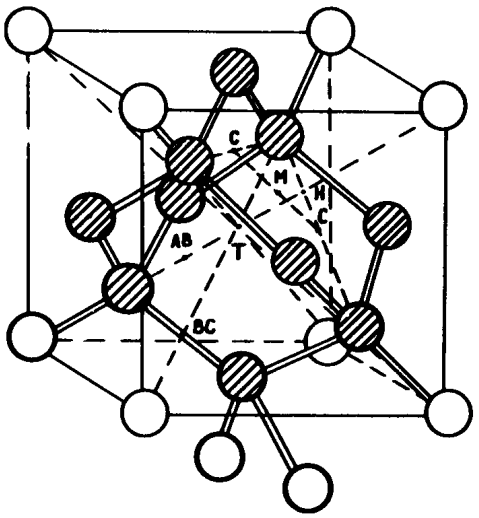

Fig. 2. Fragment of silicon lattice ○ — silicon atoms, ● — silicon atoms of Si_8H_{18} cluster, ◎ — silicon atoms of $Si_{10}H_{16}$ cluster

ters $HX_{10}H_{16}$ (X=Si,C) saturated with H atoms and centered at the tetrahedral (T) interstitial site, have been performed whereas for Mu at the BC site we used the MuX_8H_{18} clasters centered at this site (fig. 2). As shown at /5/, the model «Mu at the H site» fails to adequately describe the Mu* properties. In contrast, the properties of Mu located at the BC site are in perfect qualitative agreement with those experimentally determined for Mu*(H*).

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