



Formation of chemically bound positively charged radiation defect induced by negative muon in diamond crystals



Yu.M. Belousov ^{a,*}, L.P. Sukhanov ^{a,b}

^a Moscow Institute of Physics and Technology, 141700 Dolgoprudny, Institutskiy lane 9, Russia

^b National Research Center "Kurchatov Institute", 123182 Moscow, Russia

ARTICLE INFO

Article history:

Received 23 January 2015

Received in revised form 30 April 2015

Accepted 1 May 2015

Available online 6 May 2015

Keywords:

Diamond lattice

Negative muon

Positively charged radiation defect

Quantum-chemical calculations

Radiation transition rate

ABSTRACT

The formation process of a positively charged radiation defect bound chemically with a diamond lattice is considered. This defect originates as a result of a negative muon capture by a carbon nucleus and formation of the so called "pseudo-boron" muonic atom ${}_{\mu}\text{B}$. Numerical calculations (Antipov et al., 2012) of the neutralization kinetics of the radiation defect have shown that it lacks a time interval for neutralization during electron trapping in a track within a muon life-time $\tau_{\mu} = 2.2 \cdot 10^{-6}$ s. Therefore, there appeared a necessity for considering alternative neutralization processes. Thus, a model of the positively charged ${}_{\mu}\text{B}^{+}$ defect formation chemically bonded with a lattice, is suggested. Quantum-chemical calculations of a defect chemical bond energy with lattice atoms were carried out. Based on numerical calculations, estimates of formation rate w of the chemically bound positively charged defect were obtained, yielding $w \approx 1.7 \cdot 10^{11} \text{ s}^{-1}$. It is shown that defect neutralization is caused by the electron filling of a broken chemical bond, and this is characterized by the lattice relaxation time.

© 2015 Elsevier B.V. All rights reserved.

1. Introduction

Positively and negatively charged muons (μ^{+} and μ^{-}) are widely used for the research of condensed matter in many different areas, and for the simulation of the behavior of hydrogen-like light element impurities and chemical processes with atomic hydrogen (see, e.g., [1]). Application of muons for materials investigation has become possible due to a well developed μSR -technique based on the possibilities of supervision for a muon magnetic moment in the sample. Negatively and positively charged muons (μ^{\pm}) represent unstable leptons with a spin value of $1/2$. Negatively charged muon (μ^{-}) decays according to the scheme $\mu^{-} \rightarrow e^{-} + \nu_{\mu} + \bar{\nu}_{e}$, where ν_{μ} and $\bar{\nu}_{e}$ are muonic neutrino and electronic antineutrino, respectively. The escape probability of a decay electron depends on the angle between the electron momentum direction and the average muon spin value \mathbf{s} , thanks to what appears as a possibility to investigate local fields of a target. A muon possesses a relatively high decay time of $\tau_{\mu} \approx 2.2 \cdot 10^{-6}$ s. Such a life-time allows investigating with high precision the processes with a characteristic time $t < 10^{-5}$ s, which defines opportunities of a μSR -technique for materials property studies, well comparable with possibilities of the widely applied methods of NMR and ESR.

The behavior of μ^{+} and μ^{-} in a medium is radically different. From a chemical point of view, a positively charged muon is a light element impurity modeling a light hydrogen isotope. A negatively charged muon

ascades into the ground $1s$ -state forming a muonic atom (μ -atom). The mass of a muon equals to 207 times the mass of an electron, and therefore, its binding energy with an atomic nucleus is 207 times larger than that of an electron. After a muon capture, a large amount of energy is released, leading to the high ionization of a target atom due to the emission of Auger electrons. Further, the target Auger electrons are captured by the positively charged radiation-induced defect. Due to a high muon mass value, the negative muon screens a nuclear charge Z which is effectively becoming one unit less than Z . After defect neutralization, a replacement impurity is formed, or a muonic atom, similar to an atom isotope with a nuclear charge $Z - 1$.

This fact was well known starting from the initial stage of the muon researches (see, e.g., [2]) and gave rise to the foundation of the muon method of materials research (μSR). Systematic study of impurities' formation with a nuclear charge equal to $Z - 1$ in condensed matter was carried out at the early stages of the μSR -researches [3–5]. A muonic atom formed inside a semiconductor lattice, models an acceptor center. For example, in diamond ($Z = 6$), the negative muon, as a result of capture by a nucleus, forms a pseudo-boron, or muonic boron, which can be designated as ${}_{\mu}\text{B}$. In Si ($Z = 14$) and Ge ($Z = 32$) the negative muon is captured by a nucleus forming pseudo-aluminum ${}_{\mu}\text{Al}$ with a nuclear charge equal to $Z = 13$ and pseudo-gallium ${}_{\mu}\text{Ga}$ with a nuclear charge equal to $Z = 31$. These chemical elements are the main acceptor impurities in silicon and germanium semiconductors.

The study of acceptor center properties using μ^{-} was suggested in [6]. A possibility to extract valuable information about the hyperfine structure and interactions with a lattice of acceptor centers in different semiconductors with the help of negative muons was shown in [7–10].

* Corresponding author.

E-mail address: theorphys@phystech.edu (Y.M. Belousov).

To interpret experimental results, as a rule, one supposes that muons are thermalized in a condensed matter for a time duration shorter than the equipment resolution time. According to these suggestions, usually, while describing the muon spin polarization in a certain model, the initial time period is considered as the moment when a muon is hitting a target. However, the experimental technique development and extension of types of objects under research show that this suggestion is not always true. In particular, theoretical explanation of experimental results with positive muons in solid hydrogen and helium (see [11,12] and [13]) was successful after taking into account thermalization processes [14–16].

The recent experiments with negative muons in diamond [17–19] also show that the interpretation of the results cannot be performed convincingly under the assumption of a rapid ($<10^{-10}$ s) thermalization of the forming muonic acceptor center μB [20]. Thus, it appears actual to consider the thermalization process of a muonic acceptor center in crystals originating as a radiation-induced defect.

In this work, the formation of a chemically bound to lattice radiation defect induced by a negative muon in diamond crystals, is considered. Estimates of the rate formation of a positively charged $(\mu\text{B})^+$ center in diamond are obtained. As shown, a neutralization process of a positively charged center $(\mu\text{B})^+$ chemically bound to lattice, is determined by the lattice relaxation time. A neutralization process for radiation defects induced by a negative muon in other crystals with a diamond-type structure (silicon and germanium) was considered in [21], where there were obtained estimates of the rate of a neutral center $(\mu\text{A})^0$ formation (A is a host atom of the lattice) as a result of a radiative transition. Calculation of a thermalization rate of the radiation defect and formation of an acceptor center will be considered in the next work.

2. States of the $(\mu\text{B})^+$ center in a lattice

Simple estimates show that a substitution impurity center formed after negative muon incorporation in a *K*-shell is neutralized rapidly, capturing an appropriate number of electrons. A typical neutralization time is of the order of $t \sim 10^{-12}$ s, and the number of electrons, for example, is 5 for diamond and 13 for silicon. The muonic impurity atom formed in this process is in an excited state when its chemical bonds with lattice atoms are broken. In accordance with the standard idea of quantum chemistry, only electrons with the same general quantum number can create a chemical bond if they are on unfilled atomic energy levels, thus forming hybridized states. For lattices with a diamond structure, the electron states *ns* and *np* are represented with an equal probability, where $n = 2, 3$, and 4 relate to C, Si and Ge, respectively. Really, the hybridized states are generated within an atomic time period, but chemical bond formation is determined by exchange interactions that are weaker than coulomb interactions which form the appropriate atomic configuration.

When a chemical bond is formed, a significant value of energy (of the order of some eV) must be released. In gaseous and liquid phases, this excess energy can be transferred to a third body. In crystal, this kind of energy transfer should be inevitably connected with a phonon emission. However, a single phonon emission with an energy of ≥ 1 eV is impossible in a covalent crystal. Therefore, a transfer of such excitation energy value could be realized in case of a multiphonon process, having a small probability. Thus, the other processes should be also considered, where a radiation transition with a photon emission seems to be more preferable.

To confirm the suggestion on a fast neutralization of a radiation defect, calculations of electron capture by a charged radiation defect, formed by a negative muon in silicon and diamond crystals [21,22], were performed. The calculations in [22] have shown that the kinetics of electron capture by a positively charged radiation defect in silicon and diamond is essentially different. In silicon, a radiation defect is capturing the necessary number of electrons for a short time period $t < 10^{-10}$ s for neutralization, which confirms the qualitative estimates.

In diamond, a radiation defect captures quickly only 4 electrons, but it has not enough energy to capture the fifth electron necessary for neutralization within the muon life-time. So, in diamond, we need to consider a transition process of a positively charged radiation defect in a chemically bound state with the lattice. Hereafter, a positively charged defect chemically bound with the lattice, is neutralized as a result of the redistribution of charge carriers in the crystal valence band.

Calculations of a radiation transition rate of the neutral defect in the chemically bound state in the “main” crystals with a diamond-type structure (C, Si and Ge) in the assumption of a fast neutralization, were carried out in [21]. However, in accordance with conclusions in [22], the obtained results appear to be correct only for silicon and germanium, while for diamond it is necessary to consider the formation process of a chemically bound positively charged defect.

In accordance with the calculations of the kinetics of electron capture by a radiation defect induced by a negative muon, a positively charged impurity center $(\mu\text{B})^+$ is formed in a time duration $t \sim 10^{-12}$ s. This impurity center has the effective nuclear charge $Z = 5$, and the atomic configuration where two electrons in an external (unfilled) electron shell are not in the ground but in a “mixed” state:

$$|\psi_{in}\rangle = |2s2p\rangle. \quad (1)$$

We suppose here that the electronic configuration for the main quantum number $n = 1$ is completely filled and electronic states of the external atomic shell are described by unperturbed wave functions of a free atom. The initial state of the radiation defect in a diamond lattice is shown schematically in Fig. 1a.

The mixed state (Eq. (1)) forms a chemical bond with the nearest host atoms of the lattice. We write a wave function of the initial state (Eq. (1)) in the form of a superposition with all possible spin states:

$$\Psi_{sp}(\mathbf{r}_1, \mathbf{r}_2) = A_0 \Psi_{sp}^{(0)}(\mathbf{r}_1, \mathbf{r}_2) |0, 0\rangle + A_1 \Psi_{sp}^{(1)}(\mathbf{r}_1, \mathbf{r}_2) \sum_{M_S} |1, M_S\rangle, \quad (2)$$

where

$$\Psi_{sp}^{(S)}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} \left(\psi_{2s}(\mathbf{r}_1) \psi_{2p}(\mathbf{r}_2) + (-1)^S \psi_{2p}(\mathbf{r}_1) \psi_{2s}(\mathbf{r}_2) \right), \quad (3)$$

and $\psi_{2s}(\mathbf{r})$ is the wave function of the 2s-state. We regard that all *p*-states with different projections have equal probabilities:

$$\psi_{2p}(\mathbf{r}) = \frac{1}{\sqrt{3}} \left(\psi_{21,+1}(\mathbf{r}) + \psi_{21,0}(\mathbf{r}) + \psi_{21,-1}(\mathbf{r}) \right).$$

$S = 0, 1$ are the values of the total electron spin, and $|S, M_S\rangle$ is the appropriate spin-state vector. Spin states with different projections are considered as having equal probabilities, so, coefficients in the superposition (Eq. (2)) satisfy the following condition

$$|A_0|^2 + 3|A_1|^2 = 1.$$

The space part of the defect wave function in the final state must correspond to the determined value of the total electron spin *S*, and this can be represented in the form of superposition of hybridized states providing a chemical bond with the lattice host atoms:

$$\Psi_{Cr}^{(S)}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{6}} \sum_{\mathbf{n}_a, \mathbf{n}_b} \Psi_{\mathbf{n}_a \mathbf{n}_b}^{(S)}(\mathbf{r}_1, \mathbf{r}_2), \quad (4)$$

Download English Version:

<https://daneshyari.com/en/article/702030>

Download Persian Version:

<https://daneshyari.com/article/702030>

[Daneshyari.com](https://daneshyari.com)