Poster

THE HIGH-TEMPERATURE STABLE DEFECT CLUSTERS IN NEUTRON IRRADIATED SILICON CARBIDE: ELECTRON PARAMAGNETIC RESONANCE STUDY

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Among all known semiconductors, silicon carbide (SiC) is now facing the challenge of the material of the future. The simple evident main reason is that silicon carbide has proved its ability to be used efficiently under such extreme conditions: extreme high-temperature, high-power capabilities and high radiation conditions.

The main doping methods are ion implantation or neutron transmutation followed by high-temperature annealing. The ionic implantation and neutron transmutation doping produce unwanted damages in the SiC lattice that persist even at very high temperature. The D_1 and D_{II} centers are the best known examples of the latter type of defects in SiC which persist even at 1500^{o}C. Positron annihilation spectroscopy studies show that a wide range of vacancy aggregates are created by damage-inducing treatments in SiC.

Here we present the results of EPR study of heavily neutron irradiated (dose of 10^{21} cm^{-2}) and high-temperature annealed 6H-SiC crystals. After thermal annealing at 1500°C at least five new axially (along c-axis) symmetric centers dc-1 – dc-4 with the electron spin S=1/2 and S=1 were shown to arise in 6H-SiC crystals. The striking feature of all discovered centers is a strong hyperfine (hf) interaction with a great number (up to twelve) of equivalent host Si (C) atoms. The observed signals are marked as “dc” that is “defect cluster”. After thermal annealing at 2000°C a new triplet center labeled as N-V in the form of a silicon vacancy and a nitrogen atom in neighboring carbon substitutional position has been observed. The parameters of this center are similar to that for well-known N-V center in diamond.

Fig.1(left) shows two spectra (dc-1a and dc-1b) observed at 300K and 65K, respectively. In both spectra, there are strong central lines plus weaker satellite pairs that arise due to hf interaction of the unpaired electron of the defect with nuclear spins of adjacent Si or C atoms. The study of the intensity relation of the HF satellites to the central line allows establishing which and how many atoms contribute in the interaction. For the dc-1a signal two most intensive hf pairs with splittings of 0.65mT and 1.3mT correspond to the probability to found one and two ^{29}Si atoms among 9 equivalent Si neighbors, respectively. The most distant pair with 2.7mT splitting arises due to hf interaction with one C neighbor. For dc-1b signal two HF pairs with 1.85mT and 3.7mT splittings also arise due to interaction with 9 equivalent Si neighbors. Both signals are nearly isotropic with g = 2.0028. The hf interaction with 9Si neighbors has small anisotropy that is more pronounced for the dc-1b signal. The dashed line shows the simulated spectra. The intensities of the lines of the experimental and simulated spectra practically coincide.

Two EPR signals that correspond to the S = 1 centers both with almost isotropic g- factors of g=2.002 have been found. The values of the zero-field splitting of these centers are D=187·10^{-4}cm^{-1} and D=276.3·10^{-4}cm^{-1}. The dc-2 signal could be observed in the temperature range 20 – 300K with maximum intensity at 45K while dc-3 signal has maximum intensity at 300K and could be observed down to 200K. Both signals exhibit a hf structure that is shown for the dc-2 signal in Fig. 1(right).
Since the sample has been annealed at very high temperature of 1500^{o}C, one can exclude isolated intrinsic defects as well as divacancies as possible origin of the observed signals. The behavior of the dc-1a and 1b signals at the temperature changing, similarity of their hf

structure allow to assume that they represent the same defect in the different states (phases). Possible structure is a removed part of the tetrahedron V_{Si}-$3V_C$. One can see that this defect complex has one nearest C neighbor that will cause the strongest interaction with one C atom (dc-1a). Then, twelve Si neighbors, nine of them will give smaller interaction with 9 Si. This structure may show some temperature effects since C atom, as well as other neighbors, may actually change its positions and the wave function of the unpaired electron may be distributed in different ways, leading to two states of the dc-1 center: the low temperature dc-1b state - the wave function is mainly (32%) localized on 9 Si atoms and the high temperature state dc-1a - the wave function is mainly (8%) localized on one C atom and 9 Si atoms carry smaller part of the spin density. In both cases for S = 1/2 the charge states could be +1 or –1.

Analysis of the hf structure of the dc-2 signal allows to propose it's model as a complex of two carbon atoms that form a split interstitial antisite $(C_2)_{Si}$. There is a good probability that some of new centers could be related to the famous D_1 and D_{II} centers. The main feature of $(C_2)_{Si}$ complex is the presence of the two C atoms that will cause a strong hf interaction. Then, the nearest neighbors of these two C atoms are four C atoms that cause smaller hf interaction. At last, twelve Si atoms in the 2nd shell will cause corresponding small hf interaction. Another S=1 signal, dc-3 seems to be the same defect in another position in the SiC lattice. In the case if hf interaction would occur with one Si (Fig. 1 (right)) a pair of two antisites $(C_2)_{Si}$-Si_C could be suggested as a model for dc-2 centre.

The EPR spectra of N-V defects in the triplet state in 6H-SiC reveal strong temperature dependence. This center has an axial symmetry along c-axis. The charge state of this defect seems to be +1 compare with neutral state for N-V defects with *S*=1/2. Anisotropic hyperfine splitting due to the ^{14}N nuclei has been observed. Similar to the diamond N-V centers in SiC were produced by neutron irradiation and high-temperature annealing of the crystals containing nitrogen. It seems to consist of silicon vacancy and carbon substitutional nitrogen in the adjacent lattice cites oriented along *c*-axis.

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Figures:

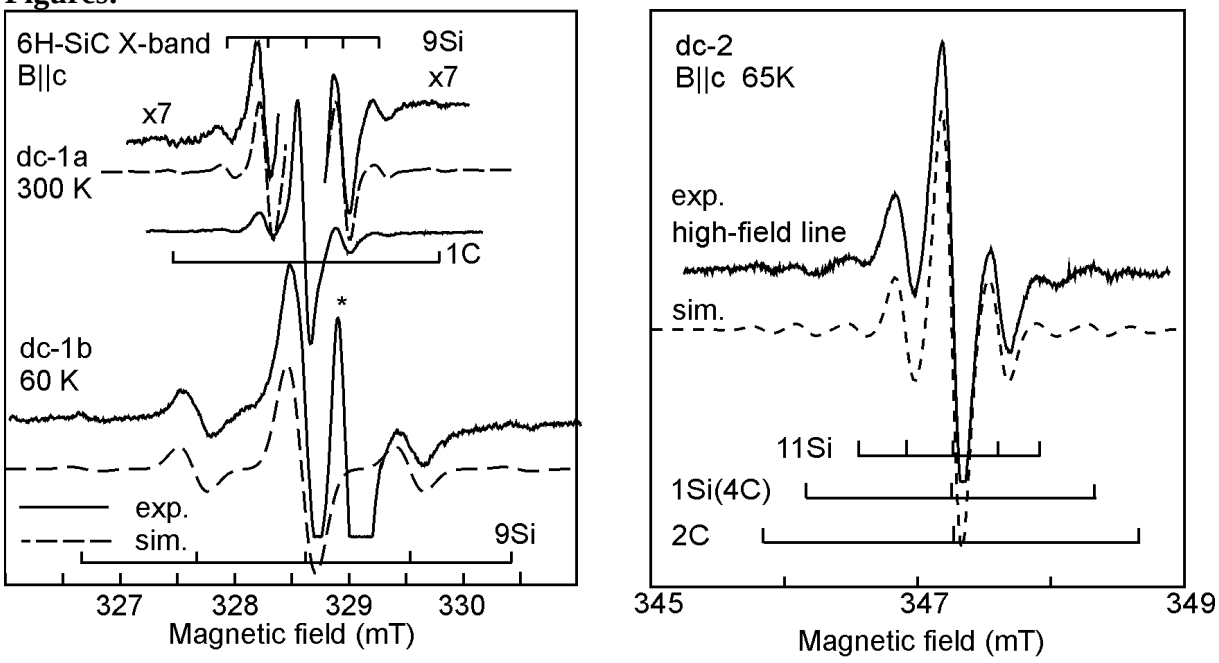

Fig. 1. Experimental (solid line) and simulated (dashed line) EPR spectra: (left) dc-1a and dc-1b centres. The hf satellites for dc-1a centre are shown with high gain; (right) high-field component of the dc-2 signal. Positions of the HF satellites are indicated