**M center in 4H-SiC is a carbon self-interstitial**

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The list of semiconductor materials with spectroscopically fingerprinted self-interstitials is very short. *M* center in 4H-SiC, a bistable defect responsible for a family of electron traps, has been deprived of a model which could unveil its real importance for almost two decades. Using advanced first-principles calculations and junction spectroscopy, we demonstrate that the properties of *M*, including bistability, annealing, reconfiguration kinetics, and electronic levels, match those of the carbon self-interstitial. [Pre-print published in Physical Review B 103, L180102 (2021); DOI:10.1103/PhysRevB.103.L180102]

The identification of self-interstitials in technological crystalline materials constitutes a rare event with profound repercussions on several fields. Together with vacancies, they form a fundamental couple playing a central role in many properties and processes, including mass transport, crystal growth, doping and countless solid-state reactions.

Silicon carbide, in particular its 4H polytype (4H-SiC), is a mainstream wide-gap semiconductor for power electronics [1, 2] and a host for some of the most promising defects for quantum technologies [3–6]. In n-type material, while both Si and C vacancies have well established spectroscopic signals accompanied by detailed models [7–13], little is known about the interstitials, apart from indirect findings from their interaction with vacancies [14, 15] and some conjectural assignments. Deep Level Transient Spectroscopy (DLTS) peaks EH, T5 [16, 17], M [18, 19] and EB [20], were to some extent related to carbon interstitials, but when the data are confronted to existing models [21–23], we only obtain a partial match. This contrasts with p-type SiC, where the connection of electron paramagnetic resonance signals T5 [24], EI1 and EB [25] to carbon self-interstitials finds support from first-principles calculations of hyperfine splitting constants, zero-field coupling coefficients [26] and g-tensor elements [27]. Of course, having reliable fingerprints of self-interstitials in 4H-SiC, and particularly in n-type material which offers better doping yield than p-type 4H-SiC, would improve our ability to control many defect engineering processes. For instance, an efficient production of quantum technological defects in n-type 4H-SiC (mostly vacancy related and invariably introduced by ion-implantation or irradiation techniques), strongly depends on our ability to control their annihilation on capturing self-interstitials during subsequent thermal treatments. This can only be achieved if we are able to follow the defects involved.

Below we demonstrate that the carbon self-interstitial (C1) is responsible for a family of DLTS traps, attributed nearly two decades ago to a defect labeled ‘M’. They show up in irradiated n-type material after moderate annealing (T ∼ 200 °C) [18, 19], including after irradiation with low-energy electrons (200 keV) [20], implying a relation to a carbon sublattice defect [28].

The *M* center is a bistable defect whose configuration is bias dependent. Spectrum labeled ‘A’, evidencing traps M1 (Ec − 0.42 eV), and M3 (∼ Ec − 0.83 eV) is obtained when the sample is cooled from room temperature under reverse bias. Conversely, when the DLTS scan is preceded by a gentle annealing at T > 140 °C without bias, spectrum ‘B’ appears, consisting of a single emission M2 (Ec − 0.63 eV) [18, 19]. The spectra can be cycled without loss of signal amplitude by repeatedly (un)biasing/annealing the sample. Since the M-peaks overlap with other prominent traps in irradiated 4H-SiC, namely Z1/2 [29] and S1/2 [30], the analysis must be carried out from differential spectra.

By applying isothermal heat treatments, it was possible to extract activation energies for the conversion between A and B configurations. In unbiased samples the B− ground state builds up at the expense of metastable A+ with an activation energy of 1.4 eV. The superscripts refer to the double minus charge state of the defect. Conversely, in reverse biased samples, the A− state recovers from metastable B− with an activation energy of 0.9 eV [18].

The reconfiguration within the neutral state could not be monitored because the B signal consisted of M2 only (B− → B− + e−). It was argued that above room temperature, a fast conversion from B− to A− frustrated the observation of an expected M4 peak related to B− → B0 + e−, effectively channeling any second emission through A− → A0 + e− [19].

Besides complying with the above observations, we show that C1 features a rich set of properties that meet those of the *M* center, such as charge states and an-
nealing. The model, developed using accurate range-separated hybrid density functional calculations combined with junction spectroscopy, includes a detailed configuration coordinate diagram (CCD).

The electronic structure calculations were based on the planewave/projector-augmented wave formalism [31] using the Vienna Ab initio Simulation Package [32, 33], where planewaves with a cut-off energy of 420 eV described the Kohn-Sham wave functions. Total energies of stable and saddle-point structures were evaluated using the density functional proposed by Heyd, Scuseria, and Ernzerhof (HSE06) [34]. Defects were inserted in 400-atom 4H-SiC hexagonal supercells whose Brillouin zones (BZ) were integrated at \( k = \Gamma \). Forces on atoms were calculated within a semi-local approximation to the exchange-correlation interactions [35] and a BZ sampling grid of \( 2 \times 2 \times 2 \) \( k \)-points. This allowed for the investigation of stable defect structures, transformation, and migration mechanisms. For the mechanisms, we used the climbing image nudged elastic band (NEB) method [36]. All forces were kept below 0.01 eV/\( \AA \). Formation energies as a function of the Fermi level were found by the usual method [37]. Spurious periodic effects were mitigated by adding a correction to the energies of charged supercells [38]. For further details and testing, see Refs. [39, 40].

Experiments were carried out on Schottky diodes fabricated on 25-\( \mu \)m-thick n-type 4H-SiC layers (nitrogen doping up to \( 4.5 \times 10^{13} \text{ cm}^{-3} \)). They were pattern-implanted through their nickel Schottky contacts with 2-MeV He ions with a fluence of \( 10^{15} \text{ cm}^{-2} \). Conventional DLTS measurements were carried out in the temperature range 100-450 K. Reverse voltage, pulse voltage and pulse width were \( V_R = -4 \text{ V} \), \( V_P = 0 \text{ V} \), and \( t_P = 10 \text{ ms} \), respectively. These conditions correspond to a depletion width of 1.7-3.5 \( \mu \)m, safely avoiding the ion projected range (4.8 \( \mu \)m). In order to stabilize the spectra and monitor structural transformations during the measurements, we applied isothermal DLTS [41, 42]. Here, 20-min-long capacitance transients were acquired at a sampling rate of 60 kHz, keeping the temperature of the samples within \( \pm 0.05 \text{ K} \) from a set-point in the range 280-340 K. Before quenching the diodes to the measurement temperature, the \( M \) centers were either set to configuration A or B by applying a –30 V reverse bias annealing at 340 K for 20 min, or annealing at 450 K for 20 min without bias, respectively.

The geometry and electronic state of \( C_1 \) in 4H-SiC strongly depends on its sublattice location and net charge, \( q \). We found four conspicuous configurations [see Fig. 1(a)], some of which are already known [21–23]. We refer to them by a sublattice site (\( k \) or \( h \)) and an index letter (a, b or c) that stands for the alignment of the C-C dimer [highlighted in black in Fig. 1(a)].

Like the analogous defect in diamond [43], neutral \( C_1 \) adopts a spin-1 state with three-fold coordinated C atoms. Two stable structures, namely \( C_1^0(h_c) \) and \( C_1^0(k_c) \), are assigned to the potential minima labeled with \( q = 0, S = 1 \), represented by a solid line in the upper part of the CCD of Fig. 1(a). Diamagnetic \( S=0 \) states are metastable, and they were found with \( h_b \) and \( k_c \) structures (dashed line in the CCD). Energies indicated below the potential minima are relative to the ground state of the respective charge state. The defect can trap up to two electrons via overcoordination of the dumbbell atoms. Negatively charged \( h_b \) and \( k_c \) (with \( q = -1 \) and \( q = -2 \)) are now stable while other geometries become unstable. NEB calculations show that \( h_c \) and \( k_c \) structures are saddle points for rotation of \( k_b \) and \( h_b \), around the \( \langle 0001 \rangle \) crystalline axis. The respective energy barriers are indicated in the CCD over the arrows that seemingly follow the potential curves. Note that \( C_1^- (k) \) and \( C_1^- (h) \) have rotation barriers as low as 0.11 and 0.24 eV. They are expected to show an effective trigonal symmetry due to thermal motion, even at cryogenic temperatures.

Figure 1(b) shows the formation energy of \( C_1 \) in 4H-SiC as a function of the Fermi level with respect to the conduction band bottom, \( E_c - E_F \). It was calculated by assuming a C-rich crystal with the carbon chemical potential obtained from bulk diamond. For the sake of clarity, line styles are connected to specific geometries (see legend) and the range of \( E_F \) values span the upper half of the gap only. Besides a charge state-dependent structure, \( C_1 \) finds its most favorable sublattice site depending on the location of the Fermi level. In n-type material (without external bias), the most stable state is \( C_1^- (k_a) \), whereas if the Fermi level is brought toward midgap (reverse bias conditions), the ground state is \( C_1^0(h_c) \). This behavior closely follows that of the \( M \) center and its spectra A and B, hereafter assigned to \( C_1(h) \) and \( C_1(k) \), respectively.

Although the charge of defects is not directly accessible by capacitance measurements, the lack of a Poole-Frenkel effect for the \( M_{1,3} \) emissions indicates that they involve acceptor transitions [19]. Directly measured capture cross-sections of the shallower \( M_1 \) and \( M_2 \) traps were about \( 5 \times 10^{-17} \text{ cm}^2 \), suggesting \( (= / -) \) transitions. The cross-section of \( M_3 \) was two orders of magnitude larger, consistent with \( M_1 \) and \( M_3 \) being two consecutive electron emissions from the same structure (spectrum A). \( M_2 \) plus a conjectured (undetected) \( M_4 \) peak would account for the analogous transitions in spectrum B. Hence, the type and number of transitions conform with the assignment of \( C_1 \) to \( M \).

The \( M \) center anneals out in the temperature range 580-640 K according to first order kinetics at a rate of \( 1.5 \times 10^{13} \exp(-2eV/k_B T) \text{s}^{-1} \), suggesting a dissociation mechanism or capture by an abundant and close trap [19]. Figure 1(c) gives the calculated Fermi energy in 4H-SiC as a function of temperature for three different nitrogen doping levels. The horizontal axis matches that of the formation energy diagram in Fig. 1(b). Considering the
SiC is a carbon interstitial. Like the carbon vacancy barrier and an entropy contribution, usually differ from the measured activation energies by a capture calculated levels neglect any temperature effects. They former agrees well with $M_2$ for forward and backward jumps $C_i^-(h_b) \leftrightarrow C_i^-(k_a)$ and $C_i^-(h_b) \leftrightarrow C_i^-(k_a)$, respectively. Both mechanisms are exothermal, and the barriers are rather close to the A $\rightarrow$ B and A $\leftrightarrow$ B conversion activation energies of 1.4 and 0.9 eV, measured without and with bias, respectively [18].

A decisive piece of evidence in the identification of the $M$ center would be a direct observation of the $M_4$ transition accompanied by $M_2$. Figure 2(a) shows DLTS spectra of a 4H-SiC n-type sample implanted with 2 MeV He ions, measured after annealing at 340 K under reverse bias (spectrum A) and 450 K without bias (spectrum B). The latter is dominated by the $Z_{1/2}$ peak (carbon vacancy) [7, 29], with relatively smaller contributions from $S_1/S_2$ (silicon vacancy) [13, 30], and a less understood broad feature known as EH$_4$, recently connected to a superposition of different alignments of anisotropic silicon vacancy structures commonly referred to as carbon-antisite-vacancy pairs [44].

It is only when we compare spectrum B with A that the presence of the bistable $M$ center becomes evident. The prominent peak at about 280 K in spectrum B is
Figure 2. (a) DLTS spectra of 2 MeV He implanted 4H-SiC SBD showing two configurations of the M center (A and B) along with other (labeled) deep traps. (b) Isothermal DLTS signals of the M center in configurations A (blue) and B (red) at 310 K. M2, M3, and M4 overlap with Z_{1/2}, S2, and EH4, respectively. (c) Differential signal (dotted curve) of the isothermal spectra shown in (b). The thin solid line represents the simulated signal from M2, M3, and M4 deep traps obtained by nonlinear fitting. See text for experimental details.

actually a superposition of Z_{1/2} with M3, the latter being converted to M1 and M3 in spectrum A (overlapping S1 and S2, respectively). As in Ref. [19] we find that above room temperature spectra A and B become identical as a result of the B → A transformation. This means that we do not have access to M center related transitions deeper than M4 (as is expected for the location of M4) by means of conventional DLTS.

Figure 2(b) depicts two isothermal DLTS spectra acquired sequentially at T = 310 K. Spectrum B was acquired first, after pre-annealing the sample at 450 K with no bias applied. During the 20-min recording time at T = 310 K, a large fraction of M centers was converted from configuration B to A. This could be confirmed from the loss of intensity of M2 during subsequent identical measurements. Spectrum A was then recorded after warming up the sample at T = 340 K under reverse bias (−30 V) in order to reset all M centers to the A form. The isothermal signals have contributions from three groups of transients: A fast group with time constant $\tau \sim 10^{-1}$ s (Z_{1/2} and M2), an intermediate group with decay time of a few seconds (S2 and M3), and a slow group in the range $\tau \sim 10^2$ to $10^3$ s (EH4 and a new peak labeled M4). The M4 peak is clearly shown in the differential spectrum of Fig. 2(c). It has the same behavior of M2 on annealing/biasing, and corresponds to a trap concentration identical to that of M1, M2, and M3 (7.8 × 10^{11} cm^{-3}).

From a fit of a $T^2$-corrected Arrhenius function to the M4 data, we obtain an activation energy for electron emission of $E_a = 0.86 ± 0.02$ eV and an extrapolated capture cross-section $\sigma_c = 4 \times 10^{-15}$ cm$^2$ which is coherent with a first acceptor transition. Although we could not directly measure the capture cross-section of M4, the agreement with the calculated $C_i^-(k_a) \rightarrow C_i^0(k_c) + e^-$ transition energy of 0.92 eV is striking. Also notable is the agreement shown in Fig. 2(c) between the isothermal data (dotted line) and its theoretical counterpart (solid line) [41], obtained via non-linear fitting constrained by the measured emission rates of M2, M3 and M4.

Unfortunately, the measurements cannot discern whether M4 is an evidence of (i) B$^-$ → B$^0$ + e$^-$ followed by B$^0$ → A$^0$ or (ii) B$^-$ → A$^-$ immediately followed by A$^-$ → A$^0$ + e$^-$. The second and first steps of (i) and (ii), respectively, are necessary to explain the gradual conversion of B into A during the isothermal transients. The calculations account for B$^0$ → A$^0$ in (i) if we consider the spin-flipping transition shown as a dashed line in the CCD. On the other hand, the first step of route (ii) has a measured activation energy of 0.9 eV, very close to the M4 emission energy, and this could reflect the rate-limiting process toward A$^0$. Regarding the C$_i$ model, although being consistent with both alternatives, this issue certainly calls for further clarification.

Another aspect that deserves a closer look, concerns the annealing mechanism of the M center. The observed first order kinetics suggests an annealing rate that depends on its own concentration only. A possible explanation stems from the indication that C$_i$ defects are most likely negatively charged during annealing, thus being Coulomb-attracted by abundant nitrogen donors. The products of such reaction could be the EB centers reported by Beyer et al. [20].

The list of alternative defects, other than C$_i$, that could be related to the M center is not long. A Si displacement is unlikely, given that M was observed in material irradiated with electrons whose energy was below the necessary displacement threshold [20]. Further, we know that the Si self-interstitial is not an acceptor and has levels considerably deeper than those of M [40].

A stronger contender is a carbon Frenkel pair. Carbon vacancies and self-interstitials have electron traps deeper
than \( \sim E_c - 0.4 \text{ eV} \). In n-type material they are both negatively charged, and Coulomb interactions between pairs with varying distances should lead to a strong dispersion of their respective trap depths. This effect is observed in DLTS spectra of as irradiated samples, but does not conform with the relatively clean M peaks, which are only visible after a gentle \((T \sim 200^\circ \text{C})\) annealing \([30, 45]\). We investigated the stability of close Frenkel pairs and found a family of markedly low-energy structures. Their formation energy is in the range 5.5-6.5 eV but the annihilation barrier is about 0.1-0.2 eV and therefore could not survive even at room temperature.

Based on first-principles calculations and junction spectroscopy, we provide substantial and credible arguments that allow us to conclude that the M center in 4H-SiC is a carbon self-interstitial. The observation of a new peak, labeled M4 and possibly connected to a previously anticipated acceptor transition, provides an important piece of evidence in the connection between M and the interstitial. The model developed is summarized in Fig 1(a) in the form of a CCD. It incorporates the observed features of M, including charge states, bistability, annealing, reconfiguration kinetics and electronic transition levels. The M center peaks are either “hidden” by the prominent Z\(_{1/2}\) signal (carbon vacancy) or by S\(_{1/2}\) (silicon vacancy) and EH\(_{1/3}\) (unidentified). While this may explain the difficulty in the identification of C\(_i\) in n-type 4H-SiC, it certainly has undermined the interpretation of defect evolution by means of DLTS, in particular during annealing. The identification of the M center in 4H-SiC as the C\(_i\) defect will contribute to a better understanding of defect-related processes, ranging from self-diffusion to the activation and migration of dopants and impurities introduced by ion-implantation.

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