Dear Editor,

We like to express our appreciation to the reviewers for their comments. We are resubmitting the revised version of the paper number SST–108576. We have studied the comments of the reviewer carefully, and have changed the text according to the comments they have listed. The location of revisions is highlighted by yellow in "Marked–SST–108576.pdf". Below we refer to each of the reviewer's comments.

Response to Reviewer #1

Comment 1. *Details that how the microwave treatments affect the semiconductors are not clear. The author claimed that it was not only heating up, and several possibilities were suggested. But still the physics of the microwave treatment is very unclear for the reviewer.*

Reply: Let's consider the possible ways microwave treatments affect defects in structures under investigation. The primary process, which determines defect production under irradiation, is a displacement of the atoms from the sites of the lattice. But the energy of a photon with frequency 2.45 GHz is about 10^{-5} eV only; the threshold displacement energies in GaAs and SiC are (8-28) eV [1] and (20-35) eV [2], respectively. Therefore such a channel of microwave-induced modification of defect subsystem is unreal.

Microwave energy is known to transform into heat inside the material. Processes based on microwave heating find many industrial applications. But the used experimental procedure (pulsed microwave radiation with a period of 500 s and a duty cycle of 1%) allowed prevention of essential heating. The calculation according to Bacherikov *et al.* [3] shows that the maximum possible heating temperature of the sample ΔT is about 1 K. The ΔT magnitude was confirmed by measurements using a T–type thermocouple. As a result, the influence of microwave heating can be neglected.

There are many experimental observations that suggest non-thermal influence of microwave fields [4, 5]. These phenomena can be related to various physical reasons. First, it is known [6, 7] that a free charged particle in an electromagnetic field performs a drift in parallel to the electric component. The drift velocity magnitude is given by $\upsilon_{\perp} \propto (E_0/m\nu)$ (where E_0 is the amplitude of the electric field, m is the mass of the particle) and velocity direction depends on the phase of the field at the initial time. Consequently, along with the systematic drift of individual charged particles, directional movement of the entire set of particles is absent. Besides, the particle drifts in the direction of wave propagation with the velocity $\upsilon_{\parallel} \propto (E_0/m\nu)^2$. However, the charged point defects in semiconductor crystal are not free and have to overcome potential barriers when moving. It can be taken into account by using effective mass m_{eff}, which exponentially depends on barrier height [7]. In our opinion, the mentioned features testify that such MW-induced movement is not responsible for revealed effects.

Second, the ponderomotive forces can arise under MW action. Under inhomogeneous microwave electromagnetic field conditions, the induced oscillatory defect fluxes are rectified, leading to directional, macroscopic mass transport [5, 8, 9]. The ponderomotive force can be described as follows [8, 7]:

$$F_p(x) = \frac{q^2\beta E_0^2}{8m_{\text{eff}}\pi^2\nu^2}\exp(-2\beta x)\,, \tag{1}$$

where q is the charge of the defect, and β is the coefficient of electromagnetic wave absorption, the axis x is along the direction of wave propagation. On the one hand, the both the MW attenuation and ponderomotive force are essential when $d \geq \beta^{-1}$ (where d is the thickness of the semiconductor crystal). On the other hand, the following expression can be used to estimate β [7]:

$$\beta = \frac{1}{c}\left(\frac{\sigma\pi\nu}{\varepsilon_0}\right)^{\frac{1}{2}}, \qquad (2)$$

where $\sigma = en\mu_n$ is crystal conductivity; μ_n is the electron mobility, 8500 cm^2/sV for GaAs, 400 cm^2/sV for SiC. Accordind to [7], the Eq. (2) is correct in the case of $(\sigma/2\pi\varepsilon_0\varepsilon\nu) \gg 1$ (where ε is the dielectric perminity; 12.9 for GaAs, 10.03 for SiC), which corresponds to the samples under investigation. The calculations show that β^{-1} is $(57-90)$ μm for SiC crystals, 138 μm for GAS2, 20 μm for GAS1 and substrate of epitaxial structures, $(100-470)$ μm for epi-layers. Thus the ponderomotive forces are able to cause the movement of the charged point defects both in the single-crystal samples and substrate of epitaxial structures, and the effect is maximal in the near–surface region. Though ponderomotive influence can not be the only reason for observed effects. In fact $\beta(\text{GAS1}) > \beta(\text{GAS2})$, however, MWT with $t_{\texttt{MWT}} = 20$ s does not lead to defect transformation in GAS1, unlike in GAS1 — see table 1. Similar results are observed for SIC1(2) and SIC3.

Third, it was shown [10, 11, 12] that under resonance conditions (the coincidence of eigenfrequencies of the dislocation segment vibrations and electrical component of the microwave radiation), multiple dislocation loops occur. Besides, the MWT causes the movement of dislocations. In particular, at $\nu = 2.45$ GHz for GaAs, resonant detachment of numerous dislocations with the length $L \leq 4$ μm becomes possible [12]. The dislocation climb is accompanied by intrinsic defect generation. In addition, the behavior of the dislocation segment in a MW electric field may be strongly affected by impurity atoms, which decorate dislocations. Having accumulated at dislocations, they, on the one hand, decrease resonance frequency; on the other hand, impurity atoms may detach from dislocations at high oscillation amplitudes, and free impurity atoms may appear in the crystal [10, 11]. In turn, the appearance of free doping atoms can result in an intrinsic defect concentration increase. In our case, the dislocation generation is confirmed by a change in both curvature radius and deformation of the near-surface crystallographic planes after MWT.

Fourth, the MW-induced destruction of impurity complexes, united in clusters, is described [10, 11, 12]. This is resonant phenomenon as well, and it is expected if the irradiation frequency is close to ion–plasma frequency $\nu_r = \sqrt{e^2 N_{\texttt{com}}/4\pi^2\varepsilon_0\varepsilon\mu}$ (where $N_{\texttt{com}}$ is the complex concentration in the cluster, μ is the reduced mass of complex ions). For example, ν_r equals to 2.01 GHz for Te^+–Cu^- complex with $N_{\texttt{com}} = 5 \cdot 10^{16}$ cm^{-3} in GaAs [10]. But since the revealed transformation of deep levels relates to intrinsic defects, this mechanism seems unlikely. Besides, data about defect clusters in the samples under investigation are absent.

In our opinion, the process of MWT influence was two-stage. Initially, the resonant movement of the dislocation segment has caused an increase in the concentration of point defects, which are mostly intrinsic interstitial atoms. The approach of primary vacancy-related defects and secondary defects under the ponderomotive forces action and subsequent defect reactions occurred at the final stage. If the time of MW processing is not long enough for an essential increase in interstitial atom concentration or effective mass transport, the defect transformation does not occur, and the energy level does not change. In this case, the modification of electron capture cross-section is able under a field of newly formed dislocations (or distant point defects).

The additional information was added to the revised manuscript (page 5, last paragraph; page 6; page 7, left column paragraph 1, 4, and 5).

Comment 2. *The author's suggested modifications of the defects are too drastic. Such the defect modifications change the deep level parameters more. For example, deep level parameters for V_Si V_C and V_C in silicon carbide have been identified by both the experiments and theoretical calculations, and their parameters are very different. The small changes in deep level parameters should be other reasons. They should be experimental errors or very small modifications of the defect structures.*

Reply: The reviewer is quite right and vacancy–related defects in silicon carbide are investigated extensively — see, for instance, [13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]. In particular, it is known [15] that 6H–SiC gives rise to 3 configurations for carbon vacancy and 6 configurations for the divacancy. The further increase in deep levels, which are relevant to one defect, are connected to the different charge states.

The defect configurations were identified by using level location in the gap. The primary indicator was the maximum agreement between determined values of $(E_c - E_t)$ and data given in previous publications (see References). If the change in $(E_c - E_t)$ after MWT has exceeded the experimental errors limit, we supposed the microwave-induced configuration change. The level locations were determined from the dependency of the TAV relaxation time versus inverse temperature with enough high precision (about 10 meV). The typical dependencies are shown in Fig. 3. In our opinion, the MWT-induced changes in deep level parameters ware not so small in most cases. For example, the $(E_c - E_t)$ changes were 70 meV and 90 meV for SIC1-3 and GAT samples, respectively. The minimal level shift, which was used as evidence of defect transformation, was 40 meV.

Comment 3. *The adopted deep level observation techniuqe is not so common, and it is difficult to judge measurement accuracy. For confirmation of the results, conventional techniques such as DLTS should be employed simultaneously.*

Reply: In fact, DLTS-related techniques, designed for deep level characterization, are numerous and most widely used. Unfortunately, we are currently unable to apply the DLTS method. But it should be noted the transverse acoustoelectric voltage (TAV) has been extensively performed to characterize variety of semiconductors and their interfaces [25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38]. The most important studies include the characterization of the interface between the GaAs and its anodic oxide, and detection of defect levels in GaAs, InP, InAs, CdS, Si crystals, $Hg_{1-x}Cd_xTel/CdTe$, ZnSe/GaAs, Si/SiO_2 heterostructures, Si MOS–structures, epi-GaAs, and $Al_{1-x}Ga_xAs/GaAs$ quantum wells [31, 25, 29, 37, 33, 32]. The principle of TAV spectroscopy closely coincides with the idea of the original DLTS technique; as a result, the names "acoustic deep-level transient spectroscopy (A-DLTS)" [26, 32, 33, 34] or "acousto-electric deep level transient spectroscopy (AEDLTS)" [35] are used this method as well. Besides, the acoustoelectric transient spectroscopy has some strengths over the original DLTS. First, DLTS requires the measurement over a wide temperature range in the case of the presence of defects, which differ significantly in a level location. TAV spectroscopy needs a much narrower temperature range. Second, the acoustoelectric transient spectroscopy does not require barrier formation. On the one hand, the rectified contact formation can influence the defect subsystem in the near-surface region before/after microwave processing. On the other hand, the presence of metal contact before irradiation significantly affects the penetration of electromagnetic waves into the semiconductor. Third, the TAV method permits the detection of traps at the epi–layer and substrate interface [36, 37, 38]. The last two features were notably essential in our case.

Comment 4. *The materials observed are not the state of the art materials in industries. Therefore, even if the results and physics are truth, the impacts of this manuscript are limited. If the microwave treatment has surely advantages compared with conventional processes, the author can apply it to industry important materials, such as 4H-SiC or GaN.*
Reply: The font was enlarged.

[39, 40, 41]

Single crystalline SiC is a suitable material for realization of high power, high frequency and high temperature devices

This study aimed Summary of the trap parameters detected by the A-DLTS in Si-MOS structures

Response to Reviewer #2

Comment 1. *I suggest the authors concentrating on a specific semiconductor, digging deeply on the evolution of defects after MWT, and discussing the effect of doping on the process. The current work relates to the type of the host, the single crystal/epitaxial layers, doping concentrations. Readers lost easily during the introduction of results and discussions.*
Reply: The text was revised.

Comment 2. *The authors carried out MWT experiments on differently doped SiC or GaAs. Did the concentration of dopants change the evolution of point defects? The Fermi level is different for differently doped hosts, which charge states of intrinsic defects and MWT-induced defects, and thus the interaction, may be different.*
Reply: The text was revised.

Comment 3. *The Pool-Frenkel effect is related to defect states of dislocations. Yes, some works dealt the interaction between irradiation-induced point defects and dislocations, such as Appl. Phys. Lett. 117, 023501 (2020) and J. Mater. Chem. C 9, 3177 (2021). But I didn't see any detailed discussion in this work.*
Reply: The text was revised.

Comment 4. *Typos throughout the manuscript should be corrected, including but not limited to:*

(1) "and semiconducting compounds including [6, 8]"
(2) "doping degree"
(3) "$0 : 31 \div 0 : 33$"

Reply:
The text was revised.

Response to Reviewer #3

Comment 1. *The reviewed manuscript presents results on investigation of deep levels in various materials before and after microwave treatment with different durations (doses). Therefore, the investigation is not well focused, since the nature of defects is different for different materials, and they not necessarily should be governed by the same trends.*
Reply: The text was revised.

Comment 2. *The results could present interest, even though the investigated materials are not the state of the art ones in industries. However, the used experimental method is not widely approved, and the identification of the microscopic nature of defects is not an easy task even with widely used investigation methods such as DLTS or DLOS. As a result, the discussions about the microscopic nature of the observed defects and their reconfiguration during the microwave treatment as well as the made conclusions are not enough convincing (especially in cases when the deep level activation energies do not change very much under microwave treatment, as well as in cases when there is a large difference between the experimental results and those coming from theoretical consideration).*
Reply: The text was revised.

Comment 3. *I consider that the manuscript is not suitable for publication in the present form. However, the reliability of the obtained results may be significantly improved, if the study is complimented with other methods of investigation such as DLTS or DLOS, at least for some of the investigated materials. Moreover, the DLTS method also gives information about the concentration of deep levels. In such a case, a comparison of parameters of deep levels obtained by TAV and DLTS, combined with an analysis of the results of previously performed investigations, may provide enough arguments confirming the proposed microscopic nature of defects and their transformations.*
Reply: The text was revised.

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