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Molecular Dynamic Simulation on Temperature Evolution of SiC under Directional Microwave Radiation

Tahsin Ashraf Khan[1*], Patrick Burr[2], David Payne[1], Mattias Juhl[1], Utshash Das[1], Brett Hallam[3], Darren Bagnall[1] and Binesh Puthen Veettil[1]

[1]*School of Engineering, Macquarie University, NSW 2109, Australia*
[2]*School of Material Science and Engineering, University of New South Wales, NSW 2207, Australia*
[3]*School of Photovoltaic and Renewable Energy Engineering, University of New South Wales, NSW 2207, Australia*

**Corresponding author*
204 Epping Road, Marsfield, NSW-2122
Email: tahsin-ashraf.khan@students.mq.edu.au
Contact number: +88 (0) 1712547651

ABSTRACT:

Silicon carbide (SiC) is widely used as the substrate for high power electronic devices as well as susceptors for microwave (MW) heating. The dynamics of microwave interaction with SiC is not fully understood, especially at the material boundaries. In this paper, we used the molecular dynamics simulation method to study the temperature evolution during the microwave absorption of SiC under various amplitudes and frequencies of the microwave electric field. Directional MW heating of a SiC crystal slab bounded by surfaces along [100] crystallographic direction shows significantly faster melting when the field is applied parallel to the surface compared to when applied perpendicular.

Keywords: *Microwave absorption, Silicon Carbide, Molecular Dynamics, Temperature Evolution, Accelerated Melting*

INTRODUCTION:

Microwave heating of materials has emerged as a fascinating research area during the past decade. El Khaled et al. (2018) showed in their work that energy exchange between microwaves and materials could be used as a viable alternative to conventional heating in some industries for thermal processing, owing to its better temperature control, volumetric, selective, and rapid heating. Although microwave heating and microwave annealing (MWA) techniques have been used in food industries since the mid-1800s, as shown in the works of Ibrahim et al. (1843), and in ceramics and rubber industries mentioned by Singh et al. (2015), they are relatively new to semiconductor processing. Alford et al. (2009) has used MWA in semiconductor and photovoltaic industries to form shallow, well-defined p-n junctions in ion-implanted silicon samples. Sarswat and Free (2013) used microwave-based synthesis of CZTS (copper zinc tin sulphide) materials for

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photovoltaic applications in the field of semiconductors. Studying MWA and obtaining consistency in results has been challenging because the heating rates depend on numerous parameters such as moisture content, changes in dielectric properties with temperature, sample size, geometry, and the strength of the electric field, as mentioned in El Khaled et al. (2018) paper. The discrepancies in temperature measurements of the volumetrically heated samples have often resulted in reporting 'non-thermal' effects of microwave heating until it was disproven recently by the brilliant work of García-Baños et al. (2019).

Silicon Carbide (SiC) assisted heating has been employed widely in the MWA applications for semiconductor processing demonstrated in the works of Kremsner and Kappe (2006), Isfort et al. (2010) and many others. With the advent of high power and high-frequency electronics, the use of SiC as the semiconductor substrate has been increasing, as pointed out in the works of Deng et al. (2020) and Nelson et al. (2020), thanks to its high power density, heat dissipation and bandwidth capability. Microwave absorption and heating in these substrate surfaces mainly depend on conductivity loss and polarisation relaxation loss as demonstrated in SiC nanotubes Gong et al. (2021) Zhang et al. (2021). The polarization loss seemed to be caused by the surface suspension bonds induced band gap reduction as observed by Yang et al. (2019), which is again observed in SiC nanowires by Jia et al. (2020).

Wang et al. (2015), Yang et al. (2014) and Liang et al. (2014) showed that SiC has also found widespread use as a susceptor material that enables secondary heating by microwave in ceramic, rubber, food and recycling industries. In both high-frequency switching applications and microwave processing applications, SiC absorbs microwaves through its intrinsic electric dipole polarization. Microwave absorption invariably results in substrate heating as seen by Cao et al. (2010), which is a desirable condition for microwave processing. As reported by Zhang et al. (2021) the real part of the permittivity has a direct proportionality with temperature, which is attributed to the shortened relaxation time of electron polarization. On the other hand, the imaginary part also increases which is ascribed to the increasing electrical conductivity of the carbon fibers in the carbon fibre/silica composite. Cao et al. (2015) and Jiang et al. (2016) experimentally demonstrated that the microwave absorption properties can be further altered by surface modification of the susceptor. However, a theoretical model for the heating dynamics of SiC with surface boundaries interacting with polarized microwave radiation is not yet reported.

Previous theoretical studies, such as WanJun et al. (2013) on SiC melting, were limited to perfect crystal structures with periodic boundary conditions and devoid of surfaces or defects. The experimentally observed variation or the jump in the heating rates of SiC for specific input MW field strengths showed by Tandon et al. (2006) could not be explained by those models. In this paper, the heating dynamics of bulk and slab SiC under polarized microwave radiation are studied using molecular dynamics (MD) simulations. The heating dynamics of SiC under polarized radiation applied perpendicular and parallel to the surface planes are also investigated.

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MODEL AND SIMULATION DETAILS:

Classical molecular dynamics (MD) has been an effective tool for mathematically modelling and simulating material interactions at the molecular level, as presented by BrooksIII et al. (2021). We used Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software created by Plimpton (2014) to perform MD simulations for this work.

Atomic interactions were described based on the interaction potential introduced by Vashishta et al. (2007), which includes three-body interactions (necessary to model the partly covalent bonding of SiC) and Coulomb forces (required to account for microwave-matter interactions). Vashishta et al. (2007) mentions the charge transfer between Si and C atoms, resulting in the Coulomb interaction between ions. This calculation of Coulomb interaction is vital to include MW induced dipole moment in the SiC substrate. The total potential energy of the system is given by:

$$V = \sum_{i<j} V_{ij}^{(2)}(r_{ij}) + \sum_{ij<k} V_{jik}^{(3)}(r_{ij}, r_{ik}) \quad (1)$$

Where V is the effective interatomic interaction potential, $V_{jik}^{(3)}(r_{ij}, r_{ik})$ represents the three-body interaction potential. The two-body interaction potential is given by,

$$V_{ij}^{(2)}(r) = \frac{H_{ij}}{r^{\eta_{ij}}} + \frac{Z_i Z_j}{r} e^{-r/\lambda} - \frac{D_{ij}}{2r^4} e^{-r/\xi} - \frac{W_{ij}}{r^6} \quad (2)$$

Where H_{ij} represents the steric repulsion between the i^{th} and j^{th} atoms, D_{ij} is the strength of the charge-dipole attraction, W_{ij} is the strength of Van der Waals interaction, and $\frac{Z_i Z_j}{r} e^{-r/\lambda}$ is the Coulomb interaction term. More details on the expressions can be found in the original work of Vashishta et al. (2007).

The bulk SiC was simulated using a 4096-atom supercell of the cubic zinc-blende structure (3C-SiC) obtained by replicating the unit cell 8×8×8 times along the three crystallographic axes, with periodic boundaries. The supercell size and structure were chosen following the published work on modelling interaction potential for SiC systems in Vashishta et al. (2007). The cubic cell size was 34.784 Å on each side, and the density was 3.2175 g/cc for the bulk. For surface calculations, 5×5×20 supercell having 4100 atoms was used instead, with a 4.345 nm vacuum on top and bottom along the z-direction, which is the [001] crystal direction. The slab contains a silicon-terminating surface on top and a carbon-terminating surface at the bottom, keeping the total number of carbon and silicon equal (2050 carbon and 2050 silicon). The simulated SiC slab was anchored to the centre of mass of the system.

All simulations were first equilibrated at 300 K using the constant pressure and temperature (NPT) ensemble for 25 ps, followed by a microcanonical (NVE) run with an alternating electric field to mimic microwave field, following the previous microwave heating studies modelled in LAMMPS by Afify and Sweatman (2018) and Wang et al. (2021). The timestep was taken as 1 fs, and the periodic boundary conditions were chosen for the systems. Since silicon carbide is a non-magnetic material, microwave interaction is dominated by the electric field. The oscillating electric field is introduced according to the following equation:

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$$\boldsymbol{E}(t) = \boldsymbol{e_n} E_0 sin(2\pi f t) \quad (3)$$

Where, E_0 is the amplitude, $\boldsymbol{e_n}$ is the direction of the electric field, *f* is the frequency, and *t* is the elapsed time of the MW radiation. The MW-material interaction is introduced by adding a force $\boldsymbol{F}_i(t) = q_i \boldsymbol{E}(t)$ to each atom *i* in the system, where *q* is the charge of the atom. For this system, charges assigned were Si = 1.201 and C = -1.201 electron charge unit according to Vashishta et al. (2007). In this study, the MW field was applied in the [100] direction for the bulk crystal and in the [100] and [001] directions for the slab. This model was tested with Vashishta potential on a (001) surface orientation slab under conventional heating and found similar melting temperature. Vashishta et al. (2007) reported the melting point of bulk SiC to be around 3200 K and the current system of layer SiC started melting at around 2700 K and completely melted at 3100K. Also the system was constrained by the center-of-mass position of the slab by adjusting the coordinates of the atoms every timestep. This ensured there was no oscillation in phase with the electric field. It is worth noting that MW radiation is "emulated" in LAMMPS by directly applying a force on atoms, i.e., we assume perfect and direct energy transfer from electromagnetic to kinetic in these simulations.

RESULTS AND DISCUSSION:

MW irradiation at 100GHz frequency with various electric field intensities (from 0.1 to 0.5 V/Å) was applied to bulk SiC to demonstrate the heating. The heating profiles (temperature *vs.* time) shown in figure 1 confirms the temperature dependence of the heating rates of SiC demonstrated in the previous studies by Tandon et al. (2006) and Zhang et al. (2014). The heating profile was approximately fitted to an exponential growth equation of the form $T(t) = T_0 e^{\beta t}$, where *T* is the temperature in Kelvin (K), *t* is the elapsed simulation time in nanoseconds (ns), T_0 is the initial temperature of the system and β is the fitting coefficient which is considered to convey the heating rates of the material.

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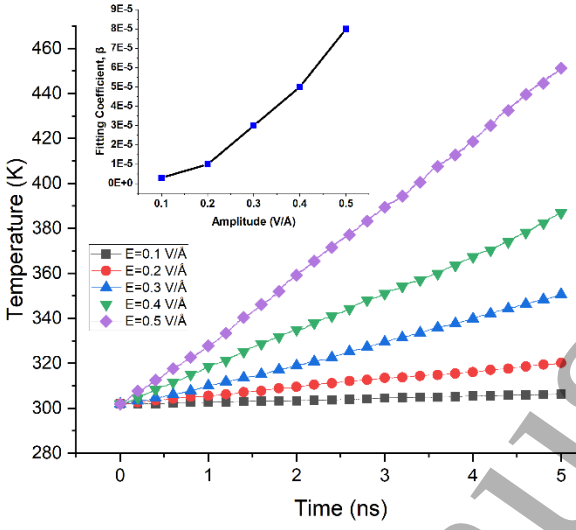

Figure-1: The time evolution of the temperature of a 3C-SiC pure bulk crystal under a 100GHz MW radiation for the first 500 periods of the wave. The inset shows the heating rate represented by the fitting coefficient, β, for various electric field strengths.

Understandably, the heating rate increases with the electric field intensity of the applied microwave due to the increase in the radiative input energy. The inset shows the impact of the electric field strength on the fitting coefficient β. A square-law relationship is observed between β and the electric field amplitude, which is expected for MW heating as showed for MW heating of water by Afify and Sweatman (2018).

Microwave heating profiles for 3C-SiC for various frequencies were extracted for constant field intensities. A 2D heat map is shown in Figure 2(a), which displays the heating profiles for microwave frequencies of 10, 50, 100, 200 and 300 GHz and amplitude from 0.1 to 0.5 for the first 500 MW radiation cycles. The fitting coefficients, β were obtained similarly for all heating profiles and were normalized for power. Figure 2(b) shows the heating rate and MW frequency relationship when the amplitude is constant at 0.5 V/Å.

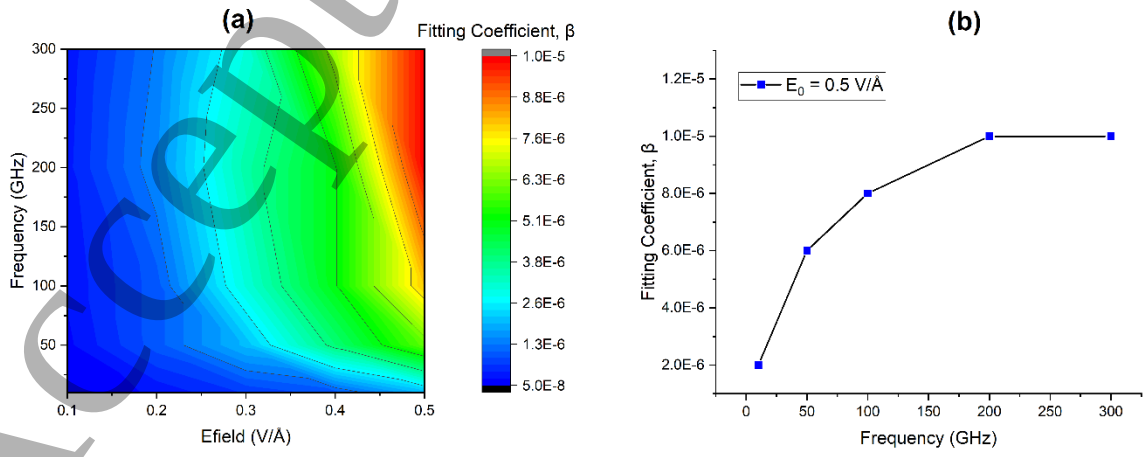

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Figure-2: (a) The 2D heat map showing the impact of electric field intensity and frequency on the fitting coefficient (heating rate) of pure bulk 3C-SiC crystal. (b) β vs Frequency when the amplitude is kept constant at 0.5 V/Å.

Fitting of the heatmap contours revealed that the relationship is accurately described by a cumulative Gaussian function (R^2=0.984) rather than the expected exponential function (R^2=0.62). This supports the finding in the previous study of Tandon et al. (2006), where it was experimentally observed that the heating profile could not be described using a single exponential function. Table 1 shows the values of the fitting parameters A and B (unitless), E (in GHz), C is in the same units as D, È is in the same units as F. Also to note that "E_{field}" represents the electric field (in Volts per Angstrom, V/Å) and "Frequency" (in GHz) of the applied MW.

Table 1: The values for Cumulative Gaussian function for β

$$\beta = A + 0.25B\left(1 + erf\left(\frac{E_{field}(\mathrm{V/Å}) - C}{\sqrt{2}D}\right)\right)\left(1 + erf\left(\frac{Frequency(GHz) - \grave{E}}{\sqrt{2}F}\right)\right)$$

Fitting Parameters	Values
A	-2.3767E-7 ± 3.5054E-7
B	2.80587E-5 ± 2.02619E-5
C	0.59385 ± 0.19825
D	0.25229 ± 0.08562
E	39.88957 ± 4.94874
F	47.54487 ± 6.17573

Directional MW with the same frequency and power was applied to the surface structure crystal along the X and Z axes (equivalent to parallel and perpendicular directions to the surface, respectively). The resultant heating profiles are compared and shown in Figure 3(a).

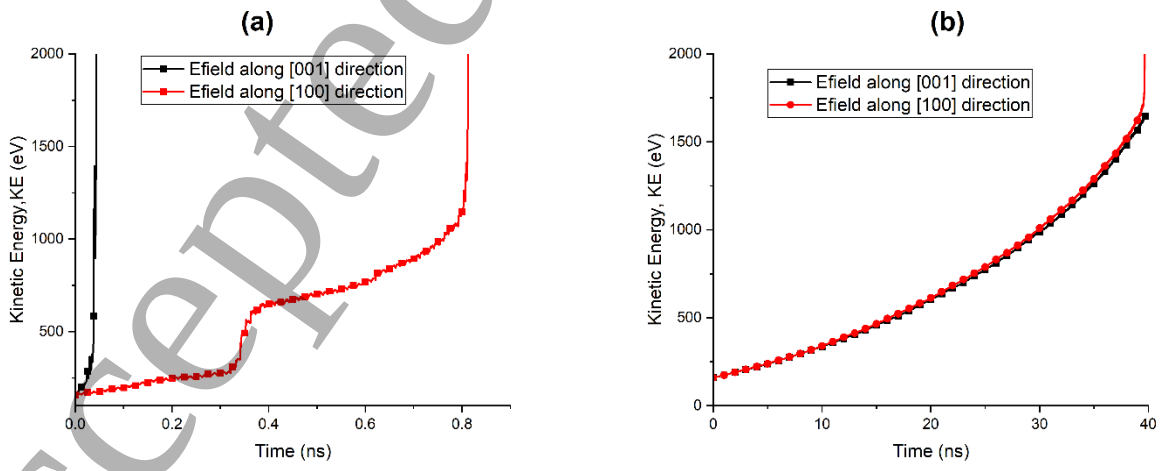

Figure-3: Time evolution of temperature of 3C-SiC (a) surface and (b) bulk when irradiated with 500 cycles of 100 GHz, 0.5 V/A microwave radiation along z-axis or [100] direction (red) and x-axis or [001] direction (black).

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MW heating in the bulk crystal, shown in Figure 3(b), demonstrates the same heating behaviour as in Figure-1 with no discernable difference in heating between the two directional microwave radiations. However in the presence of a surface, the heating dynamics heavily depend on the direction of the applied microwave.

Figure 4 shows the structural evolution of the SiC slab during heating under MW radiations parallel and perpendicular to the surface. The time-averaged kinetic energy (for every 250 fs) visualization in Figure 4 is taken for 100 GHz, 0.5V/A microwave radiation along [001] and [100] to the layered SiC.

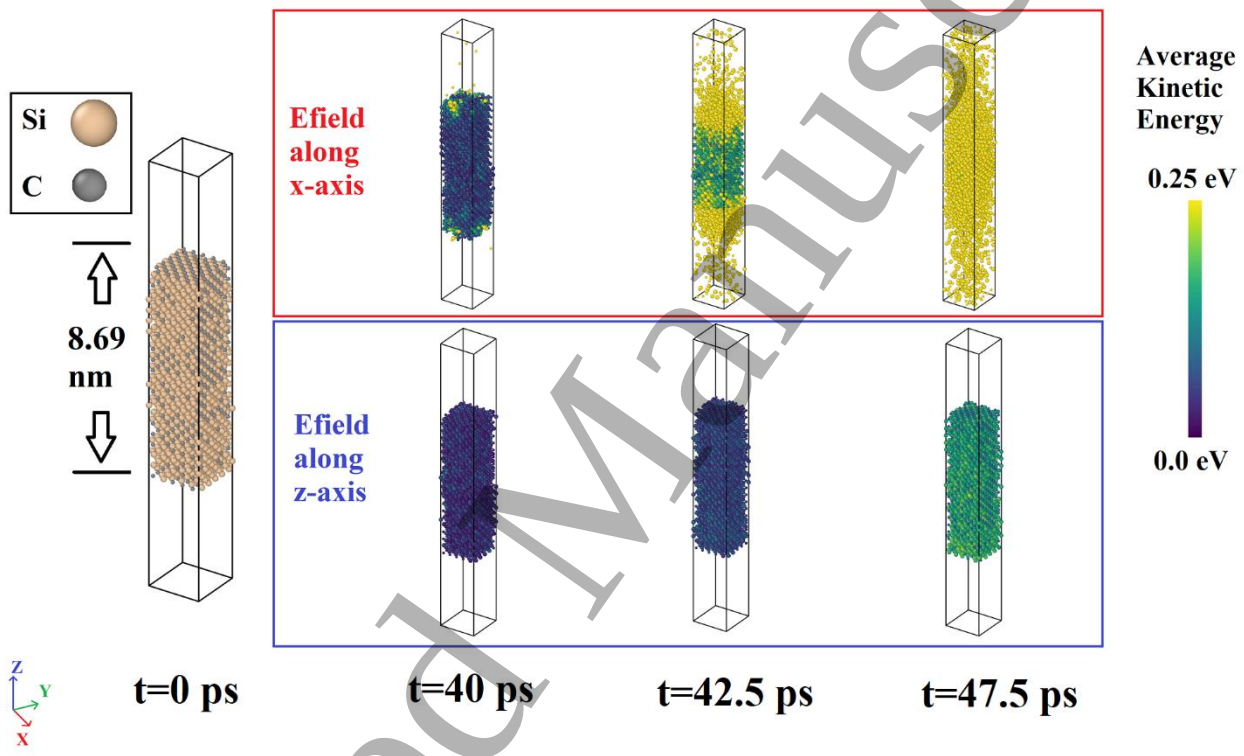

Figure-4: On the left, SiC slab with void on top and bottom along the z-axis. Snapshots in the top (E-field along the [001] direction or x-axis) and the bottom (E-field along the [100] direction z-axis) showing kinetic energies and the structural information at three different timesteps during the MW heating.

When MW radiation is applied in the [001] direction or x-axis, local melting and spallation occur near the surface, as shown in figure 4 in the snapshot at t=40 ps. The system gradually melts at the top and bottom at t=42.5 ps as more atoms are energized and finally completely melt after t=47.5 ps. Figure 4 shows hotspots near the surface, which suggests that melting initiates near the surface. The process of surface atoms initiating to break away from the crystal can be compared to random crystal growth from a seed atom within a molten substrate as such that in both cases the process is quite random. At first few atoms from the surface gets superheated and escapes into the void, creating a sharp increase in the overall kinetic energy change. The heating rate of the temperature evolution vs time curve is seen to have a "knee" formation in Figure 3(a) around that timestep. The knee formation indicates the beginning of local melting at the surface and this is observed irrespective of the MW irradiation direction. This result agrees with the previous theoretical studies

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done by Hu et al. (2017) and Phillpot et al. (1998) and experimental study done by Newman (1982). As for pure bulk SiC, "Mechanical melting" was observed, also demonstrated by Phillpot et al. (1998) in their paper. Mechanical melting is defined as a homogeneous crystal lattice breakdown (unlike thermodynamic melting, which arises around the crystal defects and surfaces) that transforms the crystal into the liquid phase within a few femtoseconds.

The bottom portion of figure 4 shows the snapshots of the system when MW is applied perpendicular ([100] direction) to the surface, which shows little to no heating compared to the corresponding parallel MW heating. The directional heating of the layered SiC system suggests that the system will melt much quicker (~20 times faster) when the MW radiation is incident parallel to the surface of the void. This phenomenon may be attributed to the nature of the surface bonds. The dangling bonds at the surface produce orientation-dependent polarization which seems to play a deciding role in the higher MW heating rate in the x-direction. Further studies on different surface orientations and terminations may reveal the impact of the surface effects on microwave heating.

CONCLUSION:

MW heating of 3C-SiC crystal was studied using MD simulations. The heating rate for the bulk SiC unilaterally increases with increasing electric field intensity, and the dependence of heating rate on the electric field and frequency shows a cumulative Gaussian behaviour and not the expected exponential behaviour. The heating profile of the defect-free bulk SiC shows no dependence on the direction of the MW radiation, whereas SiC slabs with surfaces along [100] direction show that the heating profile is direction-dependent. MW radiation applied parallel to the SiC surface caused the crystal to melt approximately nineteen times faster than MW radiation perpendicular to the surface.

Author Contributions

Tahsin Ashraf Khan: Investigation, Methodology, Writing - Original Draft. **Binesh Puthen Veettil:** Resources, Methodology, Writing, Review & Editing. **Patrick Burr:** Conceptualization, Methodology, Validation, Review & Editing. **David Payne:** Methodology, Review & Editing. **Mattias Juhl:** Methodology, Review & Editing. **Utshash Das:** Review & Editing. **Brett Hallam:** Review & Editing. **Darren Bagnall:** Review & Editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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REFERENCES:

Afify, N.D., Sweatman, M.B., 2018. Classical molecular dynamics simulation of microwave heating of liquids: The case of water. J. Chem. Phys. 148. https://doi.org/10.1063/1.5001928

Alford, T.L., Thompson, D.C., Mayer, J.W., Theodore, N.D., 2009. Dopant activation in ion implanted silicon by microwave annealing. J. Appl. Phys. 106, 114902. https://doi.org/10.1063/1.3260245

BrooksIII, C.L., Case, D.A., Plimpton, S., Roux, B., Spoel, D. van der, Tajkhorshid, E., 2021. Classical molecular dynamics. J. Chem. Phys. 154, 100401. https://doi.org/10.1063/5.0045455

Cao, M.-S., Wang, X.-X., Cao, W.-Q., Yuan, J., 2015. Ultrathin graphene: electrical properties and highly efficient electromagnetic interference shielding. J. Mater. Chem. C 3, 6589–6599. https://doi.org/10.1039/C5TC01354B

Cao, M.S., Song, W.L., Hou, Z.L., Wen, B., Yuan, J., 2010. The effects of temperature and frequency on the dielectric properties, electromagnetic interference shielding and microwave-absorption of short carbon fiber/silica composites. Carbon N. Y. 48, 788–796. https://doi.org/10.1016/J.CARBON.2009.10.028

Deng, X., Zhu, H., Li, X., Tong, X., Gao, S., Wen, Y., Bai, S., Chen, W., Zhou, K., Zhang, B., 2020. Investigation and Failure Mode of Asymmetric and Double Trench SiC mosfets under Avalanche Conditions. IEEE Trans. Power Electron. 35, 8524–8531. https://doi.org/10.1109/TPEL.2020.2967497

El Khaled, D., Novas, N., Gazquez, J.A., Manzano-Agugliaro, F., 2018. Microwave dielectric heating: Applications on metals processing. Renew. Sustain. Energy Rev. 82, 2880–2892. https://doi.org/10.1016/j.rser.2017.10.043

García-Baños, B., Reinosa, J.J., Peñaranda-Foix, F.L., Fernández, J.F., Catalá-Civera, J.M., 2019. Temperature Assessment Of Microwave-Enhanced Heating Processes. Sci. Reports 2019 91 9, 1–10. https://doi.org/10.1038/s41598-019-47296-0

Gong, P., Yang, Y.Y., Ma, W.D., Fang, X.Y., Jing, X.L., Jia, Y.H., Cao, M.S., 2021. Transport and recombination properties of group-III doped SiCNTs. Phys. E Low-dimensional Syst.

Accepted Manuscript

Nanostructures 128, 114578. https://doi.org/10.1016/J.PHYSE.2020.114578

Hu, Y., Nakano, A., Wang, J., 2017. Directional melting of alumina via polarized microwave heating. Appl. Phys. Lett. 110, 044102. https://doi.org/10.1063/1.4973698

Hu, Y., Nakano, A., Wang, J., Angeles, L., Angeles, L., n.d. Supplementary Material for " Directional Melting of Alumina via Polarized Microwave Heating" 1, 1–5.

Ibrahim, M., Rahim, R.A., Nordin, J.M., Zulaika, S., Nyzam, A., Amira, N., 1843. Dielectric properties characterization of the rice and rice weevil for microwave heating treatment.

Isfort, P., Penzkofer, • T, Pfaff, • E, Bruners, • P, Gü, • R W, Schmitz-Rode, • T, Mahnken, • A H, 2010. Silicon Carbide as a Heat-enhancing Agent in Microwave Ablation: In Vitro Experiments. https://doi.org/10.1007/s00270-010-0033-6

Jia, Y.H., Gong, P., Li, S.L., Ma, W.D., Fang, X.Y., Yang, Y.Y., Cao, M.S., 2020. Effects of hydroxyl groups and hydrogen passivation on the structure, electrical and optical properties of silicon carbide nanowires. Phys. Lett. A 384, 126106. https://doi.org/10.1016/J.PHYSLETA.2019.126106

Jiang, W., Sun, M., Zhang, K., Dai, X., Xia, Y., Wang, D., Xie, A., Wu, F., 2016. Using γ-Fe2O3 to tune the electromagnetic properties of three-dimensional (3D) polypyrrole (PPy) and its broadband electromagnetic absorber. RSC Adv. 6, 68128–68133. https://doi.org/10.1039/C6RA11235H

Kremsner, J.M., Kappe, C.O., 2006. Silicon Carbide Passive Heating Elements in Microwave-Assisted Organic Synthesis. J. Org. Chem. 71, 4651–4658. https://doi.org/10.1021/JO060692V

Liang, C., Liu, C., Wang, H., Wu, L., Jiang, Z., Xu, Y., Shen, B., Wang, Z., 2014. SiC–Fe3O4 dielectric–magnetic hybrid nanowires: controllable fabrication, characterization and electromagnetic wave absorption. J. Mater. Chem. A 2, 16397–16402. https://doi.org/10.1039/C4TA02907K

Nelson, B.W., Lemmon, A.N., DeBoi, B.T., Hossain, M.M., Mantooth, H.A., New, C.D., Helton, J.C., 2020. Computational Efficiency Analysis of SiC MOSFET Models in SPICE: Static Behavior. IEEE Open J. Power Electron. 1, 499–512. https://doi.org/10.1109/OJPEL.2020.3036034

Newman, R.C., 1982. Defects in silicon. Reports Prog. Phys. 45, 1163–1210. https://doi.org/10.1088/0034-4885/45/10/003

Phillpot, S.R., Yip, S., Wolf, D., 1998. How Do Crystals Melt? Comput. Phys. 3, 20. https://doi.org/10.1063/1.4822877

Plimpton, S., 2014. LAMMPS Features and Capabilities.

Sarswat, P.K., Free, M.L., 2013. An investigation of rapidly synthesized Cu2ZnSnS4 nanocrystals. J. Cryst. Growth 372, 87–94. https://doi.org/10.1016/J.JCRYSGRO.2013.03.022

Singh, S., Gupta, D., Jain, V., Sharma, A.K., 2015. Microwave processing of materials and

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applications in manufacturing industries: A Review. Mater. Manuf. Process. 30, 1–29. https://doi.org/10.1080/10426914.2014.952028

Tandon, R., Wereszczak, A., Lara-Curzio, E., 2006. Heating Rates of Silicon Carbide in a Microwave Field. Mech. Prop. Perform. Eng. Ceram. Compos. II 27.

Vashishta, P., Kalia, R.K., Nakano, A., Rino, J.P., 2007. Interaction potential for silicon carbide: A molecular dynamics study of elastic constants and vibrational density of states for crystalline and amorphous silicon carbide. J. Appl. Phys. 101, 103515. https://doi.org/10.1063/1.2724570

Wang, C., Liu, H., Song, L., Tan, J., Yang, W., Cheng, L., 2021. Temperature evolution, atomistic hot-spot effects and thermal runaway during microwave heating of polyacrylonitrile: A ReaxFF molecular dynamics simulation. Nano Sel. https://doi.org/10.1002/NANO.202100061

Wang, H., Wu, L., Jiao, J., Zhou, J., Xu, Y., Zhang, H., Jiang, Z., Shen, B., Wang, Z., 2015. Covalent interaction enhanced electromagnetic wave absorption in SiC/Co hybrid nanowires. J. Mater. Chem. A 3, 6517–6525. https://doi.org/10.1039/C5TA00303B

WanJun, Y., TingHong, G., XiaoTian, G., YunXiang, Q., Quan, X., 2013. SCIENCE CHINA Physics, Mechanics & Astronomy Melting kinetics of bulk SiC using molecular dynamics simulation. Sci China-Phys Mech Astron 56, 1699–1704. https://doi.org/10.1007/s11433-013-5184-4

Yang, H., Cao, M., Li, Y., Shi, H., Hou, Z., Fang, X., Jin, H., Wang, W., Yuan, J., 2014. Enhanced Dielectric Properties and Excellent Microwave Absorption of SiC Powders Driven with NiO Nanorings. Adv. Opt. Mater. 2, 214–219. https://doi.org/10.1002/ADOM.201300439

Yang, M., Zhou, W., Liu, Y., Li, L., Luo, F., Zhu, D., 2019. LiCoxNi1−xO2 with high dielectric and microwave absorption performance in X-band. Ceram. Int. 45, 17800–17805. https://doi.org/10.1016/j.ceramint.2019.05.351

Zhang, M., Cao, M.S., Shu, J.C., Cao, W.Q., Li, L., Yuan, J., 2021. Electromagnetic absorber converting radiation for multifunction. Mater. Sci. Eng. R Reports 145, 100627. https://doi.org/10.1016/J.MSER.2021.100627

Zhang, Y., Li, J.-L., Wang, X.Y., Wang, J.P., Wang, B.Z., 2014. Molecular dynamics simulation on temperature and structure characteristics of microwave-heating NaCl solution. MMWCST 2013 - Proc. 2013 Int. Work. Microw. Millim. Wave Circuits Syst. Technol. 161–164. https://doi.org/10.1109/MMWCST.2013.6814595

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