# Investigation of the Electromagnetic Properties of Silicon Carbide in the mmWave Frequency Range Using Density Functional Theory

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***Abstract*— This study uses density functional theory (DFT) to investigate the electromagnetic (EM) properties of silicon carbide (SiC). Focuses on developing a methodology bridging the gap between nanoscale and continuum modeling. Using the SIESTA program, the crystal structure of SiC is modeled. In the simulations, the influence of the electric field in two directions was checked, revealing the anisotropic behavior of the material. From the real and imaginary permittivity, the loss angle in SiC up to 450 THz was calculated with the smallest value for 72.5 GHz. Conductivity was also obtained for this particular frequency.**

***Keywords—numerical methods, multiphysics modelling, computational chemistry, SiC, material parameters, density functional theory***

## I. Introduction

Millimeter-wave materials measurements have evolved along with innovative techniques for accurately determining the electromagnetic parameters needed to model systems. A key goal is to combine continuous and ab initio modeling, with efforts by organizations such as the European Materials Modeling Council (EMMC) to integrate different approaches to achieve greater accuracy. Collecting and correlating data from different methods is thus crucial to a consistent understanding of materials properties. This involves comparing results derived from different software and methodologies, a practice essential for achieving a unified understanding of the material behavior.

Our focus in this work is directed towards extracting material parameters of Silicon Carbide (SiC) specifically for mmWave applications. The material parameter extraction method will be tested on this model. We employ Density Functional Theory (DFT) calculations, an ab initio modeling, to derive key parameters such as conductivity $\sigma$ and loss tangent $tan\delta$. As a main goal we want to integrate ab initio calculations with the continuum level, specially for use in EM simulators. This research is an integral part of our broader activities conducted within the framework of the European project I4Bags [1]. In Section II, we explain the methodology employed for solving the Kohn-Sham equations [2] within the framework of density functional theory. We expound upon the SiC model utilized and present the outcomes obtained through the employed software. At the end we present the conclusions (Section III).

## II. Methodology and Results

The methodology employed in this study is rooted in the application of Density Functional Theory (DFT). This theory simplifies the electron interaction problem by considering the electron density as the key factor governing system properties. The electron density is seen as a cloud of electrons spread throughout the system. Most of approximation used in DFT are described here [2]. A crucial role in efficient DFT calculations is played by pseudopotentials [3]. Pseudopotentials replace the interactions between electrons and nuclei, allowing for more manageable computations. The DFT calculations are performed using the SIESTA [4] program. SIESTA employs the Kohn-Sham method, allowing for the calculation of total energy and its components. The extraction of materials properties process involves two scripts included in software. The first modifies SIESTA's output file, creating an input file for material properties calculations with adjusted imaginary parts for enhanced Kramers-Kronig relations. The second one generates output files with the real and cross-checked imaginary parts of the dielectric function, a conductivity σ and $tan\delta$, as in [5]. Similar methodology is applied in here [6].

### A. Model of SiC

The model employed in this study is centered around the intrinsic semiconductor SiC crystal structure, specifically focusing on the 3C cubic polytype as depicted in Figure 1 [7]. It was chosen because of the smallest number of atoms in an elementary cell, which able us to minimalize computer effort during calculations. The fundamental characteristic of the SiC model is the bond length between Si and C atoms, which has been determined to be precisely 1.85 Å [6]. This particular bond length is crucial in understanding the structural properties and behaviors of SiC at the atomic level. To accurately represent the atom positions within the unit cell, we utilized coordinates measured in Angstroms, the same as here [8]. Whole model doesn't concern any impurities. The lattice vectors, crucial in translating the elementary cell across the entire system, were determined as follows: x = 2.12 Å, y = 1.41 Å, and z = 6.00 Å, with a lattice constant of 4.41 Å. These lattice vectors define the periodic arrangement of atoms in the crystal lattice, providing insights into the spatial arrangement of Si and C atoms in the SiC structure. The entire crystal structure of SiC used in the model was constructed based on these specified values. The crystal structure was

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rendered using the XcrySDen software [9]. The resulting visualization provides depiction of the SiC crystal structure (Fig. 1).

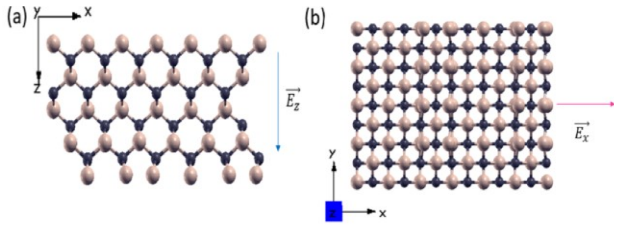


Fig. 1. SiC Structure utilized in DFT simulations: visualization in (a) Z direction and (b) XY direction of applied electric field.

### *B. Results*

The simulation framework utilized pseudopotentials for Si and C atoms, retrieved from [3]. Optical calculations were performed using a cubic mesh with 100 mesh points across each reciprocal lattice vector direction. Fig. 2 illustrates the real and imaginary parts of permittivity. Our primary interest lies in the lowest frequency ranges achievable. Due to software restrictions, the smallest energy step was utilized. For the lowest frequency, which stands at 72.5 GHz, the real part of permittivity in the z-direction is 9.96, while in the x-direction, it is 10.86. Ab initio studies on cubic SiC was already done in [11] and for 4H-SiC polytype [12]. Figure 3 presents tanδ, calculated as described in [5]. It is clear that as the frequency increases, tanδ also exhibits an upward trend. This phenomenon is particularly visible when an electric field is applied in the z- direction. Conductivity calculations were carried out, and up to a frequency of 72.53 GHz, the conductivity values are 1.24 E- 12 S/m in the z-direction and 1.732E-12 S/m in the x- direction. Above 350 THz in the z-axis direction, a phenomenon appears that requires deeper analysis due to the lack of data directly on SiC. Similar phenomena are noted for other materials [15-17].

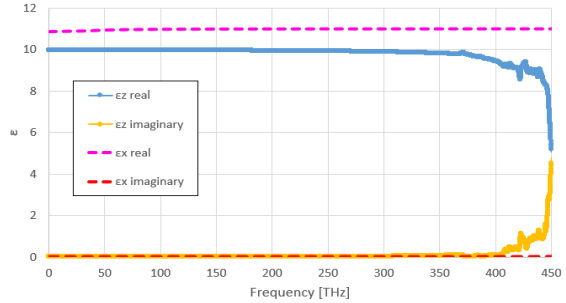


Fig. 2. The real and imaginary parts of the electric permittivity obtained for the electric field directed in the X and Z directions.

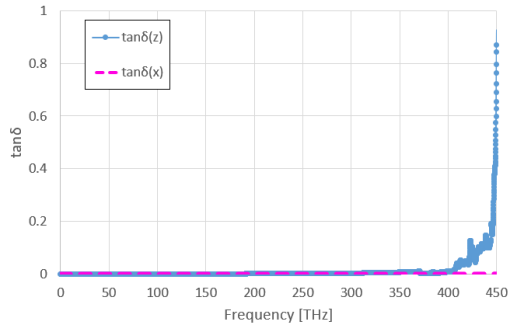


Fig. 3. The loss tangent *tanδ* obtained for the electric field directed in the X and Z directions

## III. Conclusions

In conclusion, the results obtained in this study show convergence with those reported in other publications, despite the fact that they are derived from the DFT method, which inherently involves numerous approximations. It is necessary to recognize the inherent limitations of the DFT method and emphasize the need to compare the results with established benchmarks to assess accuracy. While acknowledging the inherent inaccuracies of the method, it is crucial to emphasize its potential as a tool for gaining insights into material parameters. Going forward, our next steps include using these simulated results to derive material parameters that can be integrated into EM simulation software. This approach aims to bridge the gap between modelling. Verification of similar programs such as VASP and thorough accuracy testing is required in the future. More results will be presented at the conference.

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