Ab-initio studies of electrical and optical properties of doped diamond films: surface termination influence

B.Dec[a],R. Bogdanowicz [a],K.Pyrchla [a]

[a] *Gdansk University of Technology, Department of Optoelectronics and Metrology, Narutowicza 11/12, 80-233 Gdansk - POLAND*

e-mail: bartlomiej.dec@pg.edu.pl

In this paper, we have studied different types of calculation methods using density functional theory (DFT) in order to achieve low simulation time along with high accuracy of result. We have studied n-type and p-type diamond doped with nitrogen or boron accordingly. The particular attention was paid in this study to the boron-doped diamond films with –H, –O, -OH, -COOH surface terminations and reconstructions. The calculations were performed for doped and undoped diamond films with different crystal orientations such as (111), (110) or (100), as the most populated orientations in diamond grown in the chemical vapour deposition processes. The high accuracy relativistic pseudopotentials contained multiple projectors and semi-core states from "Open source package for Material eXplorer" were here applied. Next, the general gradient approximation with Perdew, Burke, and Ernzerhof (PBE) exchange-correlation energy as state of the art DFT functional were utilized. Achieved properties reveal that the band structure, refractive index, extinction coefficient, density of states and current-voltage characteristics show great agreement with experimental data. Such an agreement suggest that chosen methods could be used to design modified materials for advanced applications like sensors or transistors.