

Characterization of localized defect states in diamond Schottky barrier diodes fabricated on heteroepitaxial substrates

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Abstract

Diamond is a prominent wide-bandgap material with unique physical properties, including a band gap of 5.47 eV, the highest thermal conductivity of any known material, high carrier mobility for both electrons and holes, and deep chemical inertness along with biocompatibility. Due to these exceptional properties, diamond emerges as a promising candidate for the next generation of power devices. However, the limited size of seeding substrates poses challenges for the mass production of diamond-based devices. To address these size limitations, heteroepitaxial growth of diamond on foreign substrates has been introduced to facilitate larger wafers. Furthermore, the high dislocation density of the heteroepitaxial diamond substrates must be managed to improve the quality of the diamond layer and ensure the reliable high performance of diamond-based electronic devices. This thesis aims to reveal the governing parameters that influence the performance of heteroepitaxial diamond Schottky diodes. These parameters include the type, size, and thickness of the Schottky metal, along with electrical characteristics such as the ideality factor, Schottky barrier height, specific on-resistance, breakdown voltage, and thermal stability. Careful selection of the contact metal type and size, combined with optimized surface termination while managing defects and trap states, can yield desirable device characteristics. It also incorporates the innovative metal-assisted termination (MAT) technique in situ during the epitaxial growth of a heavily boron-doped active layer using hot-filament chemical vapor deposition (HF-CVD). Moreover, the uniformity and concentration of the doping profile in the unintentionally boron-doped drift layer grown by microwave plasma-assisted chemical vapor deposition (MW-CVD) are demonstrated. The effects of boron-related defects and trap centers are discussed. Machine learning algorithms were utilized to predict the reverse characteristics, such as breakdown voltage and Baliga's figure of merit (BFOM), of heteroepitaxial diamond Schottky barrier diodes (SBDs) based on their forward characteristics. Modulating these parameters leads to improved device performance, stability, and consistent reproducibility. Additionally, predictions from machine learning can reduce the need for extensive experimental investigations, lowering costs and conserving time in device optimization. This thesis demonstrates that heteroepitaxial diamond holds significant potential for power applications. It provides high blocking voltage and low on-resistance, which reduces power losses and ensures excellent thermal stability. While these attributes benefit large-scale diamond devices, additional research is crucial for fully utilizing the potential of heteroepitaxial diamond devices.