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Modification of the structure of diamond with MeV ion implantation☆☆

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ABSTRACT

We present experimental results and numerical simulations to investigate the modification of structural–mechanical properties of ion-implanted single-crystal diamond. A phenomenological model is used to derive an analytical expression for the variation of mass density and elastic properties as a function of damage density in the crystal. These relations are applied together with SRIM Monte Carlo simulations to set up finite element simulations for the determination of internal strains and surface deformation of MeV-ion-implanted diamond samples. The results are validated through comparison with high resolution X-ray diffraction and white-light interferometric profilometry experiments. The former are carried out on 180 keV B implanted diamond samples, to determine the induced structural variation, in terms of lattice spacing and disorder, whilst the latter are performed on 1.8 MeV He implanted diamond samples to measure surface swelling. The effect of thermal processing on the evolution of the structural–mechanical properties of damaged diamond is also evaluated by performing the same profilometric measurements after annealing at 1000 °C, and modeling the obtained trends with a suitably modified analytical model. The results allow the development of a coherent model describing the effects of MeV-ion-induced damage on the structural–mechanical properties of single-crystal diamond. In particular, we suggest a more reliable method to determine the so-called diamond "graphitization threshold" for the considered implantation type.

1. Introduction

Considerable effort has been devoted in recent years to the application of high energy (MeV) ion implantation in the fabrication and functionalization of diamond, in particular with the aim of developing a series of micro-devices, ranging from bio-sensors and detectors to micro-electromechanical systems (MEMS) and optical devices [1–5]. This can be achieved by exploiting the strongly non-uniform damage depth profile of MeV ions and creating specific regions where the diamond lattice structure is critically damaged. After annealing, graphitization of the buried layer is achieved whilst the remaining surrounding material is restored to pristine diamond, so that spatially well-defined structures can be created by subsequently etching away the graphitized regions [6] or advantage can be taken of the conductive properties of the graphitized regions [5,7].

In order to control the spatial extension of the graphitized layer with some accuracy, it is necessary to acquire in depth knowledge of how the diamond lattice structure is modified as a function of implanted ion type, energy, fluence, implantation temperature, annealing temperature, local stress, etc. In particular, a critical damage level N_C has been identified in the literature, above which diamond is subject to permanent amorphization and subsequent graphitization upon thermal annealing [8], although some uncertainty remains on the value of N_C and its dependence on implantation parameters (e.g. depth and/or local strain, self-annealing, etc.) [2,9–12].

A well-known effect of ion implantation in diamond is surface swelling in correspondence with the irradiated regions, due to the internal density variation in the damaged crystal, which causes a constrained volume expansion [13–15]. A detailed analysis of this effect can provide additional information on the structural modifications occurring in ion-implanted diamond. This type of study was the object of investigation in Ref. [16], where a phenomenological model accounting for saturation in vacancy density was developed, and finite-element (FEM) simulations were performed to compare numerical results with experimental surface swelling measurements. In this paper, we extend the numerical procedure to model annealing effects in ion-implanted specimens, introducing the concept of a graphitization threshold in a rigorous analysis. To validate the model, the results of simulations were compared with surface swelling profilometry measurements and with high resolution X-ray diffraction (HR-XRD) analyses.

The paper is structured as follows: in Section 2, the model for structural variation of damaged diamond is reviewed and extended to annealed specimens; in Section 3, experimental and numerical

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