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Finite element analysis of ion-implanted diamond surface swelling

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ABSTRACT

We present experimental results and numerical finite element analysis to describe surface swelling due to the creation of buried graphite-like inclusions in diamond substrates subjected to MeV ion implantation. Numerical predictions are compared to experimental data for MeV proton and helium implantations, performed with scanning ion microbeams. Swelling values are measured with white-light interferometric profilometry in both cases. Simulations are based on a model which accounts for the through-the-thickness variation of mechanical parameters in the material, as a function of ion type, fluence and energy. Surface deformation profiles and internal stress distributions are analyzed and numerical results are seen to adequately fit experimental data. Results allow us to draw conclusions on structural damage mechanisms in diamond for different MeV ion implantations.

1. Introduction

Diamond is a material of great interest for its extreme physical and chemical properties: high hardness and Young modulus, wide transparency band, chemical inertness, full bio-compatibility, etc. The implantation of high energy (MeV) ions allows the fabrication and functionalization of this material, because of its peculiar characteristic of converting the pristine crystal to significantly different structural phases (graphite, amorphous and glassy carbon) when its lattice structure is critically damaged. The strongly non-uniform damage profile of MeV ions allows the direct creation of specific regions of the material with different physical properties (i.e. electrical conductivity [1,2], refractive index [3,4], etc.) or different reactivity to subsequent processing (i.e. selective chemical etching of sacrificial layers with respect to the chemically inert diamond matrix) [5]. All of this can be exploited to fabricate a range of micro-devices, ranging from bio-sensors to micro-electromechanical systems (MEMS) and optical devices [6].

Although the role of implantation fluence has been investigated in several works [7–11] some uncertainty remains on the structural modifications occurring in diamond as a function of other relevant parameters, namely the impinging ion type, energy, implantation temperature, annealing temperature, local stress, etc. [12]. With regards to ion fluence, a critical damage level D_C has been identified in the literature above which diamond is subject to permanent amorphization and subsequent graphitization upon thermal annealing, but this value seems to depend on the depth of the damaged layer, although no specific dependence has been established [9,13–15].

One relevant consequence of the structural modifications due to ion implantation is a density variation in the damaged diamond, i.e. a constrained volume expansion which leads to surface swelling in correspondence with the irradiated region [7–11]. This mechanical effect can be exploited to deduce information regarding the structural modifications occurring in the substrate.

In the present work, we compare theoretically predicted swelling values, obtained by adopting a simple phenomenological model that uses the critical damage level as a parameter, to the experimentally measured values. The analysis is carried out using finite element model (FEM) simulations, in order to correctly take into account the complex stress state and the related deformations.

This paper is structured as follows: in Section 2, the model for surface swelling is outlined; in Section 3 the experimental procedure and the relevant results are described; in Section 4 the FEM calculations are presented and a comparison between experimental and numerical data is given.

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