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Direct measurement and modelling of internal strains in ion-implanted diamond

F Bosia[1,2,3], N Argiolas[3,4], M Bazzan[3,4], B A Fairchild[5], A D Greentree[6], D W M Lau[5], P Olivero[1,2,3], F Picollo[1,2,3], S Rubanov[5] and S Prawer[5]

[1] Department of Physics—NIS Centre of Excellence, Università di Torino, Italy
[2] Istituto Nazionale di Fisica Nucleare (INFN), Sezione di Torino, Italy
[3] Consorzio Nazionale Interuniversitario per le Scienze Fisiche della Materia (CNISM), Italy
[4] Physics and Astronomy Department, Università di Padova, Italy
[5] School of Physics, The University of Melbourne, Melbourne 3010, Australia
[6] Applied Physics, School of Applied Sciences, RMIT University, Melbourne 3001, Australia

E-mail: federico.bosia@unito.it

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Abstract
We present a phenomenological model and finite element simulations to describe the depth variation of mass density and strain of ion-implanted single-crystal diamond. Several experiments are employed to validate the approach: firstly, samples implanted with 180 keV B ions at relatively low fluences are characterized using high-resolution x-ray diffraction; secondly, the mass density variation of a sample implanted with 500 keV He ions, well above its amorphization threshold, is characterized with electron energy loss spectroscopy. At high damage densities, the experimental depth profiles of strain and density display a saturation effect with increasing damage and a shift of the damage density peak towards greater depth values with respect to those predicted by TRIM simulations, which are well accounted for in the model presented here. The model is then further validated by comparing transmission electron microscopy-measured and simulated thickness values of a buried amorphous carbon layer formed at different depths by implantation of 500 keV He ions through a variable-thickness mask to simulate the simultaneous implantation of ions at different energies.

(Some figures may appear in colour only in the online journal)

1. Introduction

Ion implantation has been widely applied to the fabrication and functionalization of single-crystal diamond, with application in diverse fields such as optics and photonics [1–8], bio-sensors [9], particle detectors [10, 11] and micro-electromechanical systems (MEMS) [12–14]. Several fabrication schemes can be implemented by exploiting light ions in the 10^2–10^3 keV energy range, whose strongly non-uniform damage depth profile allows the creation of heavily damaged buried layers which graphitize after thermal annealing, whilst the structure of the surrounding material is largely restored [15–17]. Thus, spatially well-defined structures can be created by selectively etching the graphitized regions [18] or graphitic conductive paths can be fabricated for specific applications [19, 20].

To reliably design and fabricate structures with MeV ion-beam lithography, accurate control of the spatial extension of the graphitized layer is necessary. However, the mechanisms by which the diamond lattice structure is modified by ion-beam processes are still not fully understood. This is due to the complex interplay of the various parameters involved, including implanted ion species and energy, implantation fluence and temperature, post-implantation annealing temperature, local stress—and even fundamental material properties of diamond such as tensile strength are still poorly understood [21]. It has been shown [22] that primary defects, formed in the collision cascades during ion implantation, consist primarily of vacancy and interstitial atoms. At room temperature, vacancies are immobile, but interstitials can diffuse substantially, either recombining with vacancies or moving out of the implanted region [22].

