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An analytical model for the mechanical deformation of locally graphitized diamond

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ABSTRACT

We propose an analytical model to describe the mechanical deformation of single-crystal diamond following the local sub-superficial graphitization obtained by laser beams or MeV ion microbeam implantation. In this case, a local mass–density variation is generated at specific depths within the irradiated micrometric regions, which in turn leads to swelling effects and the development of corresponding mechanical stresses. Our model describes the constrained expansion of the locally damaged material and correctly predicts the surface deformation, as verified by comparing analytical results with experimental profilometry data and Finite Element simulations. The model can be adopted to easily evaluate the stress and strain fields in locally graphitized diamond in the design of microfabrication processes involving the use of focused ion/laser beams, for example to predict the potential formation of cracks, or to evaluate the influence of stress on the properties of opto-mechanical devices.

1. Introduction

A relevant number of works has concentrated in the recent years on the application of MeV-ion-induced graphitization to fabricate and functionalize microstructures and devices in single-crystal diamond, including bio-sensors [1], ionizing radiation detectors [2,3], bolometers [4], nano-electromechanical systems (NEMS) [5,6], photonic structures [7–10] and optical waveguides [11,12]. Laser-induced graphitization has also been employed to fabricate metallo-dielectric structures [13] and ionizing radiation detectors [14] in diamond. This versatility is due to the fact that both MeV-ion and laser focused beams can locally deliver high power densities in specific regions within the diamond bulk with micrometric spatial resolution in all directions, thus creating confined regions where the diamond lattice structure is critically damaged. In these regions, annealing leads to the graphitization of the damaged structure, whilst the remaining surrounding material is largely restored to pristine diamond, so that well-defined structures can be created by selectively etching the graphitized regions [3,5–12] or taking advantage of the optical/electrical properties of the graphitized regions [1,2,4,13,14]. At significantly lower damage densities (i.e. well below the graphitization threshold), ion implantation was employed to tailor the optical properties of diamond either by modifying its refractive index [15–18] to directly write/fine-tune waveguiding structures [19] and photonic structures [20], or to induce spectral shifts in the emission of luminescent centres [21]. In all of these cases, accurate knowledge is required of the modification of the diamond lattice structure as a function of implantation/irradiation parameters and in-situ/post-processing annealing conditions, in order to exactly localize the graphitized/modified layer and predict its structural effects on the surrounding material.

As far as ion implantation is concerned, the critical damage level (D_C) above which diamond is subject to permanent amorphization and subsequent graphitization upon thermal annealing is referred to as the "graphitization threshold" [22], and its dependence on implantation parameters has been ascertained (e.g. depth and/or local strain and self-annealing) [23–27]. An observable effect of ion implantation and laser irradiation in diamond is surface swelling, due to the density variation in the sub-superficial damaged regions and the corresponding constrained volume expansion [28–30]. It is therefore possible to analyze this effect

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in order to infer the structural modifications occurring in ion-implanted diamond and the extent of the density variation. In previous studies 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 [31–33]. The use of FEM modelling requires the use of specialized software and specific expertise in the field. On the other hand, oversimplified mechanical models have often been used to calculate mechanical deformations [28] and strains [34] in ion-implanted diamond in the literature, with limited predictive capabilities. In this paper, we propose a more rigorous analytical approach to derive material swelling and internal stresses following the laser or MeV-ion irradiation of diamond, and validate it by comparing its predictions to experimental and numerical data in a number of studies.

2. Analytical model

2.1. 2D modelling of graphitic layers within the diamond crystal

Well-defined graphitic regions can be created in diamond either by MeV ion implantation followed by high-temperature annealing or by irradiation with high-power pulsed laser beams. As shown in Fig. 1, the irradiation of a crystalline structure with light MeV ions at suitable fluences generally results in the formation of a sub-superficial amorphized layer, due to the peculiar depth profile of the ionic nuclear energy loss. For a given material, the thickness and depth of the amorphized layer primarily depend on the ion species and energy, as well as implantation fluence. It is worth noting that the volumetric vacancy density reported in Fig. 1 was estimated by assuming a simple linear dependence from the implantation fluence, i.e. by multiplying the fluence by the linear vacancy density per ion λ, as generated by SRIM-2008.04 Monte Carlo simulations [35] in "Detailed calculation" mode and by setting an atomic displacement value of 50 eV [36]. It has been shown that such a crude approximation (that neglects non-linear damage effects such as defect–defect interaction and self-annealing) does not provide a physically plausible estimation of the vacancy concentration [28], nonetheless it is suitable to describe the depth and thickness of graphitized layers in samples after high-temperature annealing, provided that the correct empirical graphitization threshold is adopted [34]. Moreover, as mentioned in the previous section, the diamond layer that has been damaged above the graphitization threshold is assumed to be converted to graphite upon high-temperature (i.e. 1200 °C) annealing, whilst the remaining upper layer is assumed to have reverted to the pristine diamond phase. The latter assumption is only partially justified, since it has been established that even after high-temperature annealing, the crystal structure of implanted diamond retains a small degree of residual damage [27], as clearly observable in the electrical characterization of the material [2]. However, this effect can reasonably be neglected when considering variations in the mechanical properties [26,37].

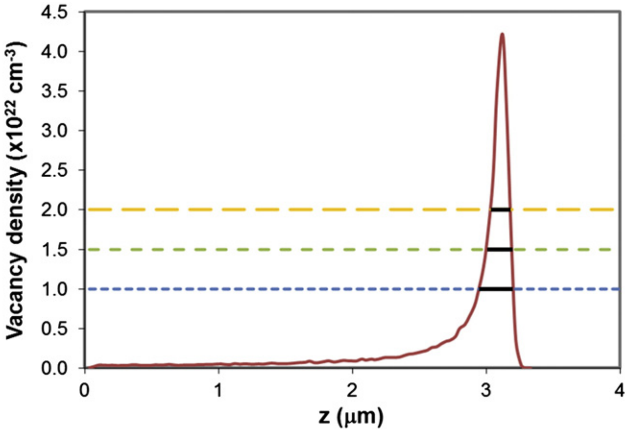

Fig. 1. Depth profile of the vacancy density induced in diamond from 1.8 MeV He$^+$ ions implanted at a fluence of 2×10^{16} cm^{-2}, as derived from the application of a linear fluence dependence to the numerical output of SRIM simulations. As an example, three critical damage thresholds are plotted (dashed lines) leading to different estimations of the thickness value h of the graphitized layer (black horizontal segments within the damage profile peak).

Although this second strategy is not considered in the present work, it is worth mentioning that extended sub-superficial graphitic layers in diamond can be obtained upon high-power pulsed laser irradiation [38,39] through non-equilibrium photo-induced phase transitions induced by fast electronic excitations that change their chemical potential [40]. In this case, a post-irradiation annealing step generally is not necessary to finalize the conversion to a graphitic phase, and the depth and thickness of the buried graphitic layer are directly determined by the extension of the region scanned by the focal point of the laser beam within the sample.

Regardless of the graphitization strategy, let us consider a diamond sample with a rectangular ion- or laser-irradiated area of length l and width w. The cross-sectional geometry of the sample is shown in Fig. 2a. The sample is modelled as a two-layer structure: a pristine diamond beam resting (with thickness t) on a graphitic elastic foundation (of thickness h), the latter undergoing a constrained expansion, due to its decrease in mass density from diamond to graphite. As a first approximation, the arbitrarily extended diamond crystal surrounding the lateral sides of the graphitic region (the "insert") is assumed to be infinitely rigid. This prevents lateral expansions, so that displacements are purely vertical (i.e. in the z direction, Fig. 2b). In order to perform an analytical study of the deformation of the diamond surface layer due to expansion of the underlying graphitic region, we employ the equation of a beam on a Winkler foundation, deriving it from the elastic beam equation [41], where the diamond and graphitic layers respectively correspond to the two above-mentioned components.

The superficial swelling of the diamond beam is thus due to the expansion of the graphitic elastic foundation because of its decrease in density. The two regions are assigned different Young's moduli (i.e. E_d for diamond and E_g for graphite), and the density decreases from the initial diamond value ρ_d to the graphite one ρ_g.

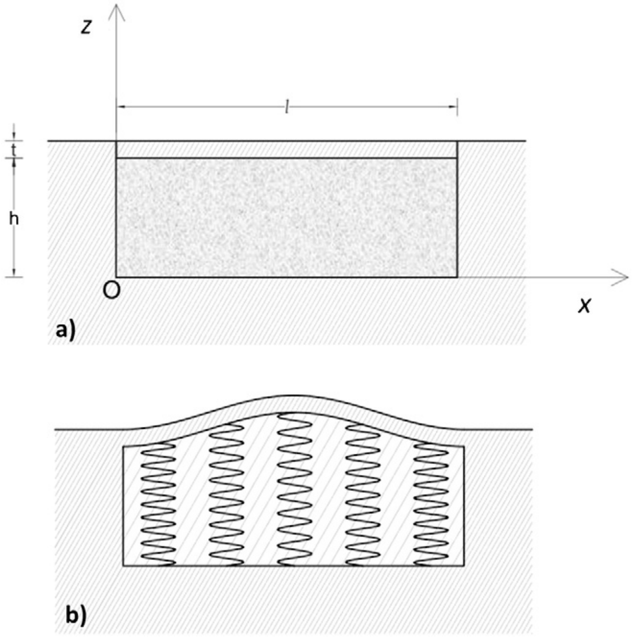

Fig. 2. a) Schematic representation of a two-dimensional section of the locally graphitized diamond region; b) deformed shape of the implanted region, modelled as an elastic foundation. The images are not to scale.