Acta Materialia 116 (2016) 95–103

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

Softening the ultra-stiff: Controlled variation of Young's modulus in single-crystal diamond by ion implantation

A. Battiato [a, b, c, d], M. Lorusso [e], E. Bernardi [a, b, c, d], F. Picollo [a, b, c, d], F. Bosia [a, b, c, d, *], D. Ugues [f], A. Zelferino [a], A. Damin [g, b], J. Baima [g, b], N.M. Pugno [h, i, j], E.P. Ambrosio [e], P. Olivero [a, b, c, d]

[a] Physics Department, University of Torino, Torino, Italy
[b] Inter-Departmental Centre "Nanostructured Interfaces and Surfaces" (NIS), University of Torino, Torino, Italy
[c] INFN – National Institute of Nuclear Physics, Section of Torino, Torino, Italy
[d] CNISM – Consorzio Nazionale Interuniversitario per le Scienze fisiche della Materia, Section of Torino, Torino, Italy
[e] Center for Space Human Robotics @ Polito, Istituto Italiano di Tecnologia, Torino, Italy
[f] Department of Applied Science and Technologies, Politecnico of Torino, Italy
[g] Chemistry Department, University of Torino, Torino, Italy
[h] Laboratory of Bio-Inspired & Graphene Nanomechanics, Department of Civil, Environmental and Mechanical Engineering, University of Trento, Italy
[i] Center for Materials and Microsystems, Fondazione Bruno Kessler, Trento, Italy
[j] School of Engineering and Materials Science, Queen Mary University of London, UK

ARTICLE INFO

Article history:
Received 23 December 2015
Received in revised form
8 June 2016
Accepted 8 June 2016

Keywords:
Diamond
Micro-/nanoindentation
Mechanical properties
Ion irradiation
Ab initio calculation
Finite element modeling

ABSTRACT

A combined experimental and numerical study on the variation of the elastic properties of defective single-crystal diamond is presented for the first time, by comparing nano-indentation measurements on MeV-ion-implanted samples with multi-scale modeling consisting of both *ab initio* atomistic calculations and meso-scale Finite Element Method (FEM) simulations. It is found that by locally introducing defects in the 2×10^{18}–5×10^{21} cm^{-3} density range, a significant reduction of Young's modulus, as well as of density, can be induced in the diamond crystal structure without incurring in the graphitization of the material. *Ab initio* atomistic simulations confirm the experimental findings with a good degree of confidence. FEM simulations are further employed to verify the consistency of measured deformations with a stiffness reduction, and to derive strain and stress levels in the implanted region. Combining these experimental and numerical results, we also provide insight into the mechanism responsible for the depth dependence of the graphitization threshold in diamond. This work prospects the possibility of achieving accurate tunability of the mechanical properties of single-crystal diamond through defect engineering, with significant technological applications, e.g. the fabrication and control of the resonant frequency of diamond-based micromechanical resonators.

1. Introduction

Diamond is an extremely attractive material for a broad range of technological applications due to its unique physical and chemical properties. In particular with regards to its extreme mechanical and thermal properties, in the past years several works were focused on developing mechanical structures and resonators in diamond either by MeV ion implantation [1,2] or by reactive ion etching [2–6] with the purpose of taking advantage of its high mechanical hardness, stiffness and thermal conductivity. Moreover, diamond hosts a wide variety of luminescent defect centres [7,8] that can act as stable single photon emitters at room temperature or as optically addressable solid-state spin-qubits [9,10]. A challenging goal in this field is to efficiently couple negatively charged nitrogen-vacancy centres to resonant mechanical structures [11–13]. For advanced applications in nano-opto-mechanical devices, the prospect of being able to modify and finely tune the mechanical properties of diamond is therefore particularly appealing. In the case of other carbon-based materials (e.g. carbon nanotubes, fullerenes or graphene), the effect of structural defects on their macroscopic mechanical properties has been studied both experimentally [14,15]

* Corresponding author. Physics Department, University of Torino, Via Giuria 1, 10125, Torino, Italy.
E-mail address: federico.bosia@unito.it (F. Bosia).

http://dx.doi.org/10.1016/j.actamat.2016.06.019
1359-6454/