Biomedical prostheses coated by tailored MWPECVD nanocrystalline diamond films

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Abstract

Different aspects concerning the use of nanocrystalline diamond (NCD) film, as coating for biomedical prostheses, is discussed. An overview is done on diamond implementation in prostheses, on the NCD mechanical properties and on the technological aspects concerning the NCD growth process i.e. Microwave Plasma Enhanced Chemical Vapor deposition. Then, the attention is focused on a possible improvement of NCD growth on titanium (Ti) substrate. Further, a theoretical study by finite element method is discussed in order to model the adhesion properties of a NCD layer on Ti and Ti/Titanium Carbide (TiC) substrates. The goal of the proposed work is to provide a study about the use of thin NCD coating on Ti based prostheses. The function of the NCD coating on Ti material is to improve the implanted prosthesis with a long duration time, thus decreasing the total costs and the invasive surgery treatments.

Introduction

Diamond coatings have been already proposed in different patents where prosthetic joints integrate diamond-coated load bearing surfaces. Polished microcrystalline diamond (MCD) coatings are utilized to reduce friction and to increase the useful life of the joint [1], or replace plastic (such as Ultra High Molecular Weight Poly-Ethylene)/ceramic (such as ZIRALLOY, which is of zirconium stabilized with magnesium) materials suitable for ginglymous, enarthrodial implants or digital joints [2]. Super hard bearing and articulation, including a prosthetic hip joint having polished MCD has been proposed by Pope et al. (2001) [3]. Nanocrystalline diamond (NCD) coated silicon nitride has been considered as a total hip replacement material in femoral prostheses [4]. Moreover, aseptic loosening and therefore the wear-debris–induced periprosthetic bone loss are the main issues for total long-term hip replacements. Amorphous diamond (a-D) coatings have been proposed to reduce the wear debris for articulating surface [5]. Results of recent studies on NCD coatings applied to medical implants have shown the high biocompatibility and positive bioactivity [6]. In alternative, multilayered NCD and MCD coatings have been studied in order to improve the hardness and the wear-resistance for articulating surfaces of structural implant devices [7].

Many properties of NCD films have been studied, in particular, the Young modulus and density of NCD films as a function of the growth time [8], the measured NCD Poisson ratio [9], and the NCD thermal expansion coefficient [10]. Moreover, friction coefficient of NCD has been measured by a proper tribosystem in different fluids [11]. In order to consider NCD film as coating material for actual prostheses, Ti is considered as substrate material. Carbon diffusion phenomena represent one of the main problem for microwave plasma enhanced chemical vapor deposition (MWPECVD) growth of diamond on Ti substrates (due to the different thermal expansion coefficients). During the growth, possible titanium carbide (TiC) layers of hundred of μm thick could be generated on the substrate interface [12] thus changing drastically the surface mechanical properties. In order to avoid this problem the working MWPECVD growth conditions described by Askari et al. (2007) [13] will be considered. In the specific study, the authors have used a high nucleation density achieved by a proper ultrasonic pretreatment (ultrasonic seeding for 60 min in a bath of ethanol with diamond powder of 30-40 μm grain size), and a moderate deposition temperature (550-600 °C which could decrease the diffusion coefficient of C in Ti and enhance the interfacial adhesion). Askari et al. (2007) [13] found an extremely thin TiC interlayer between titanium substrate and the NCD coating.

In this work, we investigated tailored, biocompatible and smoothed NCD coatings on silicon substrate produced by MWPECVD technique [14]. The low temperature (650 °C) NCD coatings exhibited the superior hardness and Young's modulus [15]. An example of topography of NCD surface obtained by the Atomic Force Microscopy (AFM) is shown in Fig. 1 where the image illustrates the small dimensions of the grains and a good surface smoothness (root main square roughness R_{RMS} = 40-60 nm).

Future depositions are planned on Ti substrate. For this purpose, the focus of the next section is devoted to understand by means of a bi-dimensional finite element method (FEM) model how a TiC layer contributes on the NCD/Ti adhesion

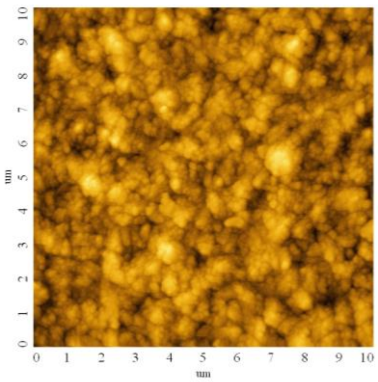

Fig.1: AFM topography image of NCD coating grown by MWPECVD.

FEM Modelling: NCD Film Adhesion Applying Loads

For a multilayered structure, the motion characteristics of the layer at the interfaces define the material adhesion (governed by adhesion energies which are strongly affected by thermal vibrations and interface roughness fluctuations). Moreover, friction mechanics depend on the friction force (F_f) at interface. The friction force is defined as $F_f = SA + \mu F_n$ where S is the adhesion shear strength, A is the contact area, μ is the friction coefficient and F_n is the normal force [16].

During the growth of a thin film on a rigid substrate, the film, constrained by the substrate, expands thus leading to the development of compressive stresses that are strong for diamond films [17]. The compressive stresses at the interface may generate film buckling and crack phenomena that change the adhesion properties of the film. The NCD film adhesion was modeled to simulate and to study theoretically the Ti/TiC/NCD multilayer by the 2D domain.

Figure 2 shows the mechanical 2D FEM modeling of NCD/TiC/Ti multilayered structure, together with the number of the triangular FEM meshes enough to simulate thicknesses of the order of 0.5 μm. By applying loads on the left and upper sides of the *x-y* spatial domain (see red arrows in Fig. 2), it is possible to model shear forces useful for the simulation of the effect of a pin-on-disk tribometer configuration [18] (measurement of the friction coefficient for a free surface). The adhesion model of 1 μm tick NCD film grown on Ti or Ti/TiC substrate is performed by setting the boundary conditions that are free boundaries for the NCD layer and fixed boundaries for the Ti layer. The interlayer boundary indicated by dashed green line in Fig. 2 represents the prescribed displacement constraint along the *x*-direction (R_x). The prescribed displacement allows to define the translational degrees of freedom of a boundary, and consequently could simulate buckling de-adhesion at the interlayer boundary by assuming different values (simulating different de-adhesion characteristics due to possible different growth working conditions).

Figure 3 shows the trends of the maximum displacement versus R_x for Ti (10 μm x 1 μm)/ NCD (10 μm x 1 μm) and for Ti (10 μm x 1 μm)/ TiC (10 μm x 0.5 μm)/ NCD (10 μm x 1 μm) multilayers by applying loads of 10 N/m. The values of Young modulus, Poisson ratio, thermal coefficient expansion, density reported in the references [8-10] were utilized for the simulation of NCD coating. The prescribed R_x values have been varied from 0 (good adhesion) to 10^{-12} m (bad adhesion). Although the presence of TiC is not wished, its thickness could be tailored by changing the growth parameters. Very thick TiC layer inhibits the NCD formation, whereas very thin layer promotes the NCD deposition and its adhesion as predict by the calculated results.

Some examples of displacement in the two limit cases of R_x= 0 m and R_x= 10^{-12} m are illustrated in Fig. 4, proving the good and bad adhesion, respectively. Studies on the variation of TiC thickness are under investigation.

Conclusions

The proposed study suggests the use of nanocrystalline diamond as coating material for human prostheses. FEM simulations highlight that 0.5 μm thick TiC can improve the adhesion of 1 μm tick NCD coating. The authors are planning to measure the friction coefficient of NCD film grown on a Si substrate by a proper tribometer system and to optimize the experimental conditions for the NCD growth on Ti substrate, to monitor the TiC thickness. The main goal is to fabricate small parts coated by NCD that may be easily integrated in the actual prostheses to improve the mechanical properties.

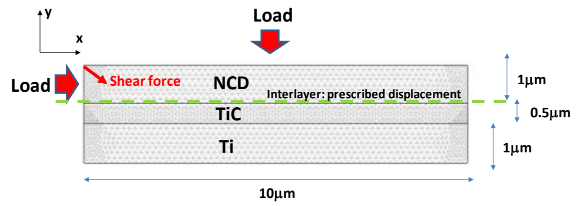

Fig.2: Mechanical 2D FEM modelling of NCD/TiC/Ti multilayered structure.

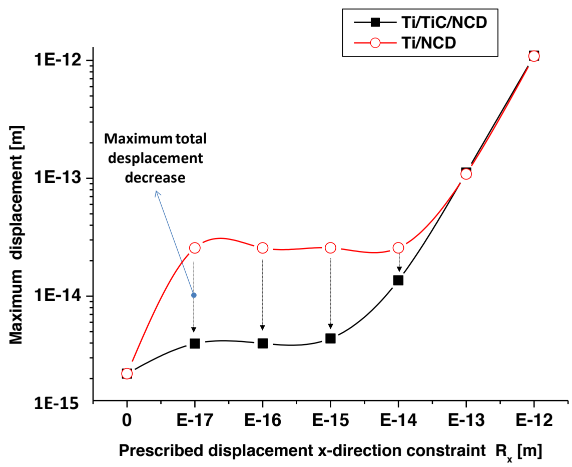

Fig.3: Maximum total displacement versus R_x for Ti/TiC/NCD e Ti/NCD multilayered structures.

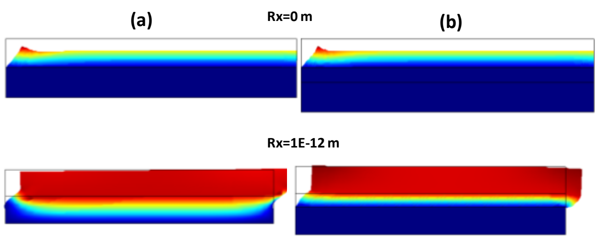

Fig.4.: Coatings displaced by applying loads on (a) Ti/NCD and (b) Ti/TiC/NCD. The 2D FEM deformations refer to R_x = 0 m and R_x =10^{-12} m.

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