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Architectural design of diamond-like carbon coatings for long-lasting joint replacements

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ABSTRACT

Surface engineering through the application of super-hard, low-friction coatings as a potential approach for increasing the durability of metal-on-metal replacements is attracting significant attention. In this study innovative design strategies are proposed for the development of diamond-like-carbon (DLC) coatings against the damage caused by wear particles on the joint replacements. Finite element modeling is used to analyze stress distributions induced by wear particles of different sizes in the newly-designed coating in comparison to its conventional monolithic counterpart. The critical roles of architectural design in regulating stress concentrations and suppressing crack initiation within the coatings is elucidated. Notably, the introduction of multilayer structure with graded modulus is effective in modifying the stress field and reducing the magnitude and size of stress concentrations in the DLC diamond-like-carbon coatings. The new design is expected to greatly improve the load-carrying ability of surface coatings on prosthetic implants, in addition to the provision of damage tolerance through crack arrest.

1. Introduction

For people afflicted with end-stage arthritis, the replacement of joints by prosthetic materials has made a great improvement to their life quality. Demand for joint replacements is rising worldwide with 1.5 million procedures performed annually worldwide [1], driven primarily by an increase in the number of joint problems associated with population aging and obesity. To lower adverse impact on the individual recipient and society, it is important that artificial joints are durable and can last for the extent of the patient's life. CoCrMo alloys have excellent mechanical characteristics [2] and metal-on-metal (MoM) bearings made of this type of alloy are used in about one third of the primary total hip replacement procedures performed in the U.S. [3]. However, MoM joint replacements are not immune to degradation in service, caused by wear and corrosion [1]. For example, the Australian National Joint Replacement Registry issued alerts for one type of MoM hip replacement in 2010, because of its high early failure rate caused by wear particles. To address this problem and significantly extend the operational lives of hip prostheses, extremely hard, low-friction coating materials have been considered for protection of joint bearing couples in recent years [4,5]. In the case of the stem portions where osseointegration is required, the bioactive coatings are utilized, which could be constituted by hydroxyapatite [6] or bioglass [7–9], and the coating layer here could be either dense or porous. These bioactive coatings are applicable to both metal and ceramic prosthetic devices. Among various coating materials tested for joint bearings, diamond-like carbon (DLC) has raised many expectations as it combines an ease of film deposition, high hardness, low coefficient of friction, and good biocompatibility [5,10–13]. Moreover, the mechanical properties of the DLC coating can be tailored by varying the ratio of sp2/sp3 bonds in its structure through the control of deposition parameters [14]. However, contact-induced cracking and delamination of the DLC coatings on metal substrates remain an issue in a biological environment [4,15]. These damages produce wear debris, which can induce catastrophic damage to the coating layer and the failure of prosthetic implants.

Different alternatives were pursued in order to combat wear damages to the coatings. For example, coatings on CoCrMo alloys with different microstructures were fabricated, resulting in a significant increase in hardness and wear resistance [16]. Two design strategies have attracted much attention in enhancing the damage resistance of hard coatings [17]. They include: a) multilayer structures, which typically contain alternating high and low modulus sublayers and b) functionally graded structures. The coating systems containing these features are capable of lowering the stress levels [18,19] and enhancing their damage tolerance. In comparison, multilayer systems have a distinct advantage over continuously graded design [14], that is, the former is capable of arresting cracks at the sublayer interfaces and hence prevents them from spreading [20,21]. However, to date no effort has been made for combining these useful features into the DLC coating for protection of MoM joint replacements.

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In the present study, an innovative modulus-graded, multilayer structure was proposed to enhance the durability of the DLC coating used in artificial joints. Finite element modeling (FEM) was applied to simulate wear particle induced stress fields in the coatings engineered on MoM bearing hip replacements. The roles of structural layering and modulus gradients in reducing stress concentrations and preventing crack initiation were examined and clarified. The material design principle demonstrated in this work suggests a new route for the design of durable load-carrying coatings for MoM joint replacements.

2. Simulation method

A ball-in-socket configuration is used in the model construction. It consists of a ball of 14 mm in radius [22] fitted into a cup; both are made from a CoCrMo alloy. Three types of DLC coatings comprising 1, 3 and 5 sublayers, respectively, are placed on the surface of the ball. All the three coating structures have the same thickness — 4 μm, which is commonly used in commercial joint replacements [23]. For the multilayer coatings a gradient in elastic modulus is applied, with the outermost layer having the highest elastic modulus, i.e., 500 GPa. Each sublayer has a constant elastic modulus, and the modulus gap between neighboring sublayers is set to be equal when moving towards the substrate. With the increase of the number of coating layers, the modulus interval decreases. Structural and mechanical characteristics of these coating systems are given in Table 1 [24,25]. In the models wear particles appear between the cup and the ball. Experiments have shown that these particles usually assume a spherical shape with the radius ranging from 2.5 to 10 μm [26].

COMSOL Multiphysics software is used to simulate the stress field induced by wear particles in these coatings. 2D axial symmetric models are constructed to reduce computational time without compromising accuracy. In these models the coating is perfectly adhered to the substrate and the interfaces between different layers are perfectly bonded. The wear particle, sandwiched between the cup and the ball, is modeled as a spherical indenter pressing onto the coating that protects the ball. Due to the fact that the ball is a spherically symmetric solid, except for the base area, which is far away from the loading zones, the loading direction applied in this work is selected for both modeling convenience and generality. The bottom boundary is fixed in the z direction to simulate the effect of the support. The rest of the boundaries are free to move. The mesh is refined within the contact region of and is further refined in the multilayer coatings, as indicated in Fig. 1. The deformation of the CoCrMo substrate is modeled in an elastic–plastic manner, characterized by a bilinear kinematic hardening stress–strain curve [24].

3. Results and discussion

Three types of cracks are often seen in hard coatings deposited on ductile substrates following indentation. They are ring, radial, and lateral cracks (also known as delamination) [27]. Ring cracks initiate at the contact edge of the indentation, and are presumably induced by high local tensile stresses. Radial cracks usually appear at the coating/substrate interface directly below the indenter under excessive radial or hoop stresses. Lateral cracks can occur under large shear stress during the loading process [28].

Table 1
The material properties used in the simulation [24,25].

Coating structure	1 layer	3 layers			5 layers				
Layer no.	1	1	2	3	1	2	3	4	5
DLC elastic modulus (GPa)	500	500	400	300	500	440	380	320	260
DLC Poisson's ratio				0.33					
CoCrMo elastic modulus (GPa)				200					
CoCrMo Poisson's ratio				0.3					

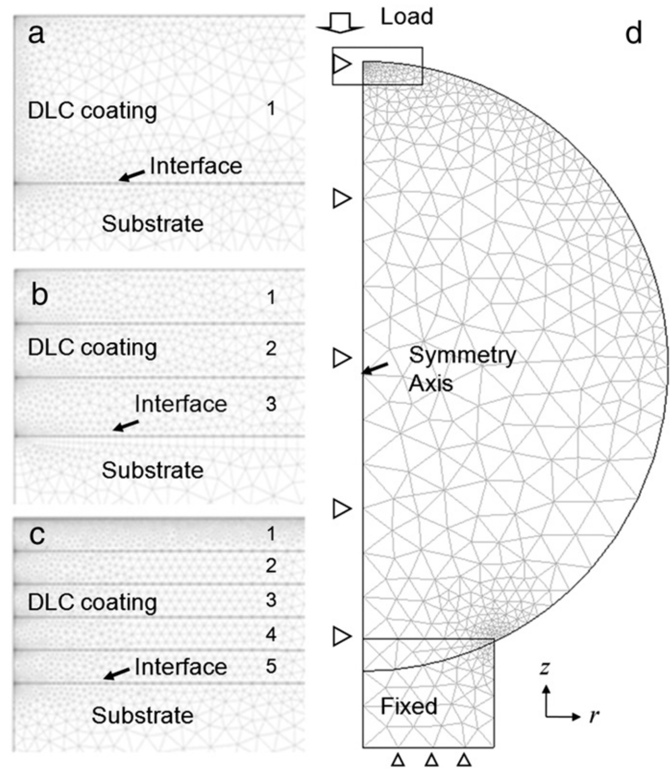

Fig. 1. Meshes used in the finite element models for (a) single layer coating, (b) three layer coating and (c) five layer coating on a CrCoMo substrate. (d) The overall model configuration used in the FEM simulation.

Typical radial stress distributions, σ_r, generated by wear particles of different sizes in three different coating structures at the indentation depth of 0.5 μm, are shown in Fig. 2. For these coatings the maximum tensile stress always appears at the interface between the coating and the substrate, along the axial symmetry axis, where radial cracks might form [29]. Local maximum tensile stress also appears around the indentation edge, where ring cracks may occur. In the case of the monolithic coating system, the magnitude and distribution of the tensile stress changes with both the indentation depth and the wear particle size. For the same wear particle size, the larger the indentation depth is, the greater the tensile stress will be induced (Fig. 3a). For example, for the particle having a radius of 10.0 μm a 350% increase in the maximum tensile stress is observed when the indentation depth increases from 0.25 to 0.75 μm. On the other hand, if the indentation depth is fixed, the larger wear particle size tends to result in lower tensile stress (Fig. 3b). Considering that the indentation strain can be defined as a/R [30], where a is the contact radius and R is the radius of the indenter (i.e., wear particles), the modeling result is consistent with the classic stress–strain behavior of materials; the greater stress is usually coupled with the larger strain.

In addition to Fig. 2, the ability of the graded, multilayer structure in lowering the maximum tensile stress is also demonstrated in Fig. 3c–e, where the radial stress distribution along the axial symmetry axis is displayed. Notably, by using 5 layer coating system, a reduction of up to 8 GPa can be achieved for a 0.5 μm indent by a wear particle of 2.5 μm in radius (Fig. 3c).

An overall comparison of results obtained from different coating systems under different loading conditions are presented in Fig. 4. The maximum radial tensile stress reaches ~30 GPa near the coating/substrate interface, when a wear particle of 2.5 mm in radius is pressed on the monolithic coating system to a depth of 0.75 μm. Note that the hardness of the DLC coating on CoCrMo substrate can reach 43 GPa [25]. Following the empirical rule that the hardness of a material is about three times its strength [30,31], the strength for the DLC coating