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Nanostructured titanium-based materials for medical implants: Modeling and development

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ABSTRACT

Nanostructuring of titanium-based implantable devices can provide them with superior mechanical properties and enhanced biocompatibity. An overview of advanced fabrication technologies of nanostructured, high strength, biocompatible Ti and shape memory Ni–Ti alloy for medical implants is given. Computational methods of nanostructure properties simulation and various approaches to the computational, "virtual" testing and numerical optimization of these materials are discussed. Applications of atomistic methods, continuum micromechanics and crystal plasticity as well as analytical models to the analysis of the reserves of the improvement of materials for medical implants are demonstrated. Examples of successful development of a nanomaterial-based medical implants are presented.

Contents

Abbreviations: ABAQUS, commercial finite element software; ARB, accumulative roll bonding; CP, crystal plasticity; DFT, density functional theory; ECAP, equal channel angular pressing; ECAP-C, equal channel angular pressing – conform; FE, finite elements; GB, grain boundary; HE, hydrostatic extrusion; HPT, high pressure torsion; GGA, generalized gradient approximation; LDA, local density approximation; MCA, movable cellular automata; MD, molecular dynamics; MLPs, martensite lattice parameters; $\mathrm{MTLS_{MAX}}$, maximum martensitic transformation; MUBINAF, multicomponent bioactive nanostructured films; NEGB, non-equilibrium grain boundary; PDA, post-deformation annealing; RSEM-RVE, representative volume element (micromechanics of materials); PIRAC, powder immersion reaction assisted coating; $\mathrm{RRS^{PC}}$, lattice strain resource recoverable strain; SEM, scanning electron microscopy; SPM, scanning probe microscopy; SPD, severe plastic deformation; TEM, transmission electron microscopy; UFG, ultra fine grained; UMAT,VUMAT, ABAQUS user subroutines; VPSC, visco-plastic self-consistent model; TJR, total joint replacements; XRD, X ray diffraction.

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1. Introduction

Due to rapid changes in the age structure of the world's population, an increasing number of people need their failed tissues to be replaced by artificial implantable devices. Metallic materials (primarily titanium and cobalt chrome alloys) are widely used for surgical prostheses, such as joint replacements, mechanical heart valves and dental implants. Although conventional materials technology has resulted in clear improvements in implant performance and longevity, rejection or implant failures still happen. The increase in average life expectancy, as well as rapid advances in modern surgery require new generations of clinically relevant biomaterials, with enhanced biological and mechanical performance. Advances in titanium manufacturing technologies are expected to play an important role in the development of the next generation of medical implants.

As forecast by a US Industry Study [1], titanium and titanium alloys will provide the best growth opportunities among biocompatible metals in the years to come and will extend applications in joint replacement systems, dental implants, fusion cages, stents, mechanical heart valves, etc.

Nanostructuring by different processing techniques is one of the promising directions in the development of Ti-based biomaterials with advanced properties. Computational modeling and numerical testing can partially replace the expensive, time- and labor-consuming mechanical and biological experiments and bring nanostructured Ti-based materials closer to clinical realization.

2. Titanium as a material of choice for medical implants

For many decades, metallic biomaterials have been used extensively for surgical implants due to the good formability and high strength and resistance to fracture that this class of materials can provide. The important disadvantage of metals, however, is their tendency to corrode in physiological conditions, and a large number of metals and alloys were found unsuitable for implantation as being too reactive in the body. Therefore, the list of metals currently used in implantable devices is limited to three main systems: iron-chromium-nickel alloys (austenitic stainless steels), cobalt-chromium-based alloys, and titanium and its alloys [2,3].

The advantages and drawbacks of metals used for implant fabrication are presented in Table 1. From the point of view of corrosion resistance, Ti is superior to other surgical metals, due to the formation of a very stable passive layer of TiO_2 on its surface. Ti is intrinsically biocompatible and often exhibits direct bone apposition. Another favorable property of Ti is the low elastic modulus (twofold lower compared to stainless steel and Co–Cr), which results in less stress shielding and associated bone resorption around Ti orthopedic and dental implants. Furthermore, titanium is more light-weight than other surgical metals and produces fewer artifacts on computer tomography (CT) and magnetic resonance imaging [4–7].

The static and fatigue strengths of titanium, however, are too low for commercially pure titanium (cp-Ti) implants to be used in load-bearing situations. The addition of alloying elements, such as aluminum and vanadium, allows for a significant improvement of the mechanical properties of titanium. Currently, Ti–6Al–4V is the most widely used surgical Ti alloy. Despite the excellent passivity and corrosion resistance of Ti–6Al–4V, elevated concentrations of metal ions were detected in the tissues around the implants, as well as in serum, urine, and remote tissue locations [8]. This slow passive dissolution and accumulation of Al and V ions has long aroused concerns regarding the long-term safety of Ti–6Al–4V alloy implants. Aluminum is an element involved in severe neurological, e.g. Alzheimer's disease, and metabolic bone diseases, e.g. osteomalacia, whereas vanadium ions were shown to be potentially cytotoxic [9,10]. Moreover, accelerated release of Al and V ions is expected to occur in tribocorrosion situations, due to the simultaneous action of corrosion and wear [11]. Given their inadequate wear resistance, Ti alloys are not used in conditions of sliding contact, e.g. in articulating components of total joint replacements. In many clinical situations, however, such as femoral stem/ball contact of modular implants, stem/bone interface of cementless implants or dental implant/bone interface, enhanced release of Al and V ions from Ti–6Al–4V can take place due to fretting (tribocorrosion involving micromotions). Therefore, much effort is being directed toward the development of V- and Al-free Ti alloys. The research on titanium alloys composed solely of non-toxic elements has been under way for several years [12].