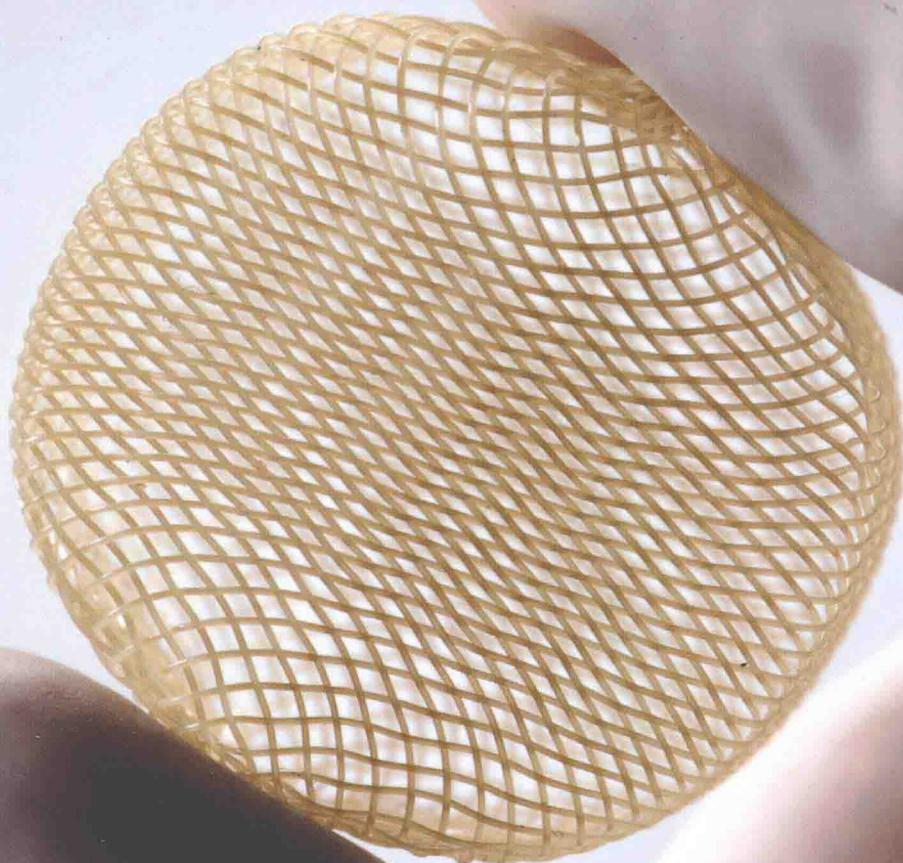


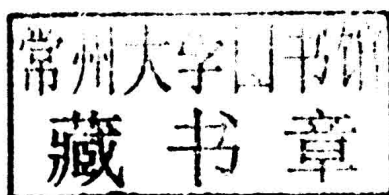
Advances and
Diverse Applications of
Biomaterials

Ralph Seguin



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Edited by **Ralph Seguin**



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Advances and Diverse Applications of Biomaterials

Preface

This book compiles reviews and original researches conducted by experts and scientists working in the field of biomaterials, covering a broad range of topics, from design to new applications. It offers readers the potentials of distinct synthetic and engineered biomaterials. This book elucidates different features of biomaterials and studies techniques used to produce biomaterials with the specific properties required for certain clinical and medical functions. It covers various topics like latest methods for characterization and evaluation of new materials, traditional applications in nanotechnology and tissue engineering, and new applications of these products. This book will be helpful for readers interested in this field.

This book has been the outcome of endless efforts put in by authors and researchers on various issues and topics within the field. The book is a comprehensive collection of significant researches that are addressed in a variety of chapters. It will surely enhance the knowledge of the field among readers across the globe.

It is indeed an immense pleasure to thank our researchers and authors for their efforts to submit their piece of writing before the deadlines. Finally in the end, I would like to thank my family and colleagues who have been a great source of inspiration and support.

Editor

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Characterization of Novel Biomaterials

Biomedical Applications of Materials Processed in Glow Discharge Plasma

V. Tereshko, A. Gorchakov, I. Tereshko,
V. Abidzina and V. Red'ko

Additional information is available at the end of the chapter

1. Introduction

There is exhaustive literature about interactions of charged particles with solid surfaces [1, 2]. For a long period only high energies were assumed to cause any significant modifications. However, low-energy ion bombardments (up to 5 keV) of metal and alloy samples were shown to be very efficient too: the increase of dislocation density (up to 10 mm in depth from the irradiated surface) was detected [3–7]. In fact, a bulk long-range modification of materials in the glow discharge plasma (GDP) took place. The above results were obtained by the use of transmission electron microscopy for well annealed samples with initially small dislocation density (armco-Fe, Ni3Fe, *etc.*) [4, 6]. For materials with initially increased dislocation density (unannealed copper, M2 high-speed steel, titanium alloys) reorganization of dislocation structure is the most considerable: either intensive formation of the dislocation fragments or grinding of the fragments with corresponding increase in their disorientation is observed. These reorganizations also take place well below the irradiated surface. When the ion energy decreases by 1 keV, the modified layer became even deeper [7].

The above results can only be explained by taking the nonlinear nature of atom interactions into account. The ion bombardment is assumed to induce nonlinear oscillations in crystal lattices leading to self-organization of the latter. Modelling shows the formation of new collective atom states. The observed phenomena include the redistribution of energy, clusterization, structure formation when the atoms stabilizes in new non-equilibrium positions, localized structures, auto-oscillations, and travelling waves and pulses [3–7].

The next step was to look at the influence of low-energy GDP on liquids. Water that occupies up 70 percent of the Earth's surface and is the main component of all living things

was taken for investigation. Water molecules are able to create molecular associates using Van der Waals forces as well as labile hydrogen interactions [8–11]. Owing to hydrogen bonds molecules of water are capable to form not only random associates (one having no ordered structure) but clusters, i.e. associates having some ordered structure [9–11]. The network of hydrogen bonds and the high order of intermolecular cooperativity facilitate long-range propagation of molecular excitations [12, 13]. This allows, in principle, to consider water and water-based solutions as systems sensitive to weak external forces. Indeed, the study of luminescence at long time scale shows that the structural equilibrium in water is not stable: it changes after dissolution of small portions of added substances and after exposition of aqueous samples to UV and mild X-ray irradiation [14].

The results obtained by Lobyshev, *et al* opened up the new avenues to water and aqueous solutions as non-equilibrium systems capable of self-organization [14]. The key property of self-organization is, however, nonlinearity to which, in models of water, hasn't paid the required attention yet. The present paper is aimed to cover this flaw. Basic models of nonlinear chains that can be related to water structure were investigated. We observed self-organization processes resulting in the displacement of atoms and their stabilization in new positions, which can be viewed as the formation of water clusters.

In experiments, we exposed crop seeds, baking yeast and water to GDP. The results were very promising: the seed sprouts showed greater growth and the yeast showed greater metabolic activity compared to the control samples. The results on volunteers with different diseases, who either drunk the processed water or was injected intravenously with the processed physiological solution, were encouraging too. The diagnostics of volunteers' blood immune cells (lymphocytes and leukocytes) showed significant normalization of their state toward homeostasis.

Next part of this paper is devoted to the study of properties of implants processed in GDP. The modern medicine is characterized by active introduction of high technologies to clinical practice. It requires sufficient biocompatibility of implanted mechanical, electromechanical and electronic devices with natural tissues. The properties of materials are crucial, since insufficient biocompatibility can lead to the negative reactions to the implant from the side of surrounding tissues causing inflammatory processes, dysfunction of the endothelium, disturbance of homeostasis, destruction and the necrosis of bone tissue and so forth [15, 16]. The formation of hydrophilic coatings and the modification of chemical composition and topography of the implant surface make it possible to reduce the frequency of the development of negative processes. The bone, fibrous and endothelial tissues are uniquely structured, and the attempts to design the next generations of implants are focused on the development of unique nanotopography of the surface of implants based on the imitation of nature. Our and other studies showed the effectiveness of vacuum-plasma technology for improving biocompatibility and durability (mechanical and chemical) of implanted materials [17–19]. New avenues in the application of above technology to the titanium implants and their influence to surrounding tissues are explored in this paper.

2. Modelling atomic and molecular chains

Molecular dynamics were used to develop the model. To describe the atomic and molecular interactions, Morse (1) and Born-Mayer (2) potentials were chosen [2].

Morse potential takes the form

$$U(r) = J \left\{ \exp[-2\alpha(r - r_0)] - 2\exp[-\alpha(r - r_0)] \right\} \quad (1)$$

where J and α are the parameters of dissociation energy and anharmonicity respectively; $\Delta r = (r - r_0)$ is the displacement from an equilibrium.

Born-Mayer potential takes the form

$$U(r) = T \cdot e^{-\frac{r}{a}} \quad (2)$$

where T , a , and r are the energy constant, the shielding and atomic lengths respectively.

We assume the existence of multiple equilibria corresponding to thermodynamic as well non-thermodynamic branches. Expanding the potentials in a Taylor series (up to the fifth order term), find the interaction force

$$F = -\frac{dU(r)}{dr} = -K\Delta r + A\Delta r^2 - B\Delta r^3 + C\Delta r^4 - D\Delta r^5 \quad (3)$$

For the Morse potential

$$\begin{aligned} K &= 2\alpha^2 J, \quad A = 3\alpha^3 J, \quad B = 2.3\alpha^4 J, \\ C &= 1.25\alpha^5 J, \quad D = 1.1\alpha^6 J \end{aligned} \quad (4)$$

where K , A , B , C , D are the coefficients of elasticity, quadratic cubic, fourth and fifth orders nonlinearities respectively.

For the Born-Mayer potential

$$K = \frac{T}{a^2}, \quad A = \frac{T}{2a^2}, \quad B = \frac{T}{6a^4}, \quad C = \frac{T}{24a^5}, \quad D = \frac{T}{120a^6}. \quad (5)$$

The coefficient values are presented in Table 1.

Coefficient	Born-Mayer potential	Morse potential
K, N/m	$9,341 \cdot 10^4$	$1,140 \cdot 10^4$
A, N/m ²	$1,951 \cdot 10^{15}$	$8,244 \cdot 10^{14}$
B, N/m ³	$2,716 \cdot 10^{25}$	$3,046 \cdot 10^{25}$
C, N/m ⁴	$2,836 \cdot 10^{35}$	$7,980 \cdot 10^{35}$
D, N/m ⁵	$2,370 \cdot 10^{45}$	$3,385 \cdot 10^{46}$

Table 1. Coefficients for Morse and Born-Mayer potentials.

There are many models that describe water molecules [13]. The molecular structure of water is presented in Figure 1. The covalent and hydrogen bonds are marked by the grey springs and the bold lines respectively. For simplicity, in our simulations we consider a chain, i.e. 1D lattice, of water molecules (see the marked area of Figure 1).

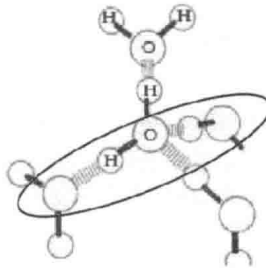


Figure 1. Molecular structure of water in a solid phase. The ellipse marks a piece of 1D chain used in simulations.

Considering only single component of $r = (x, y, z)$, say x , and viewing the atom as interacting nonlinear oscillators, the system equations take the form:

$$\begin{aligned}
 m \frac{d^2 x_1}{dt^2} &= -K' x_1 + A x_1^2 - B x_1^3 + C x_1^4 - D x_1^5 + K(x_2 - x_1) - \\
 &- A(x_2 - x_1)^2 + B(x_2 - x_1)^3 - C(x_2 - x_1)^4 + D(x_2 - x_1)^5 - \beta' \frac{dx_1}{dt}, \\
 m \frac{d^2 x_i}{dt^2} &= -K(x_i - x_{i-1}) + A(x_i - x_{i-1})^2 - B(x_i - x_{i-1})^3 + C(x_i - x_{i-1})^4 - \\
 &- D(x_i - x_{i-1})^5 + K(x_{i+1} - x_i) - A(x_{i+1} - x_i)^2 + B(x_{i+1} - x_i)^3 - C(x_{i+1} - x_i)^4 + \\
 &+ D(x_{i+1} - x_i)^5 - \beta' \frac{dx_i}{dt}, \\
 m \frac{d^2 x_n}{dt^2} &= -K(x_n - x_{n-1}) + A(x_n - x_{n-1})^2 - B(x_n - x_{n-1})^3 + C(x_n - x_{n-1})^4 - \\
 &- D(x_n - x_{n-1})^5 - K' x_n + A x_n^2 - B x_n^3 + C x_n^4 - D x_n^5 - \beta' \frac{dx_n}{dt},
 \end{aligned} \tag{6}$$

where x_i , $i = 1, \dots, n$ is displacement of i -th oscillator from the its equilibrium position, K' is the coefficient of elasticity on the chain borders, and β and β' are the damping factors inside the chain and on its borders respectively. The system (6) was solved by the Runge–Kutta method.

Relaxation processes of atoms after stopping the external influence were under investigation. Sources that gave impulses to atoms of the chains were both direct ion impact on the first atom of the chain (single impact) and random impacts on randomly chosen atoms of the chain (plasma treatment). In practice the atom bonds are important to keep unbroken, so all types of influences were low-energy ones.

2.1. Hydrogen atom chain

We carried out the simulations for chain consisting of 50 hydrogen atoms (Figure 2). Morse potential was chosen; N_i defines the number of i -th atoms. For single impact the first atom of the chain was displaced with velocity $V = 500$ m/s, which corresponds to 10^{-3} eV of the exposed energy. In case of plasma treatment the following atoms were exposed to low-energy impacts: atom N_1 ($V = 538$ m/s), atom N_{10} ($V = 1682$ m/s) and atom N_{30} ($V = 1237$ m/s).

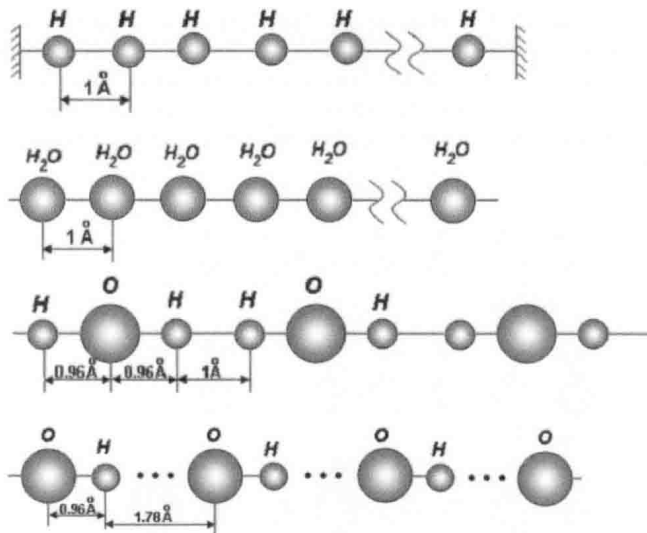


Figure 2. Chain of hydrogen atoms.

Figure 3 illustrates the atom displacements after the plasma treatment. The atoms are stabilized in the new positions that can be described as (nano)clusters (atoms N_{1-29} and N_{30-50}). After atom relaxation the simulations were continued fourth times longer, and the persistent stabilization was always observed.

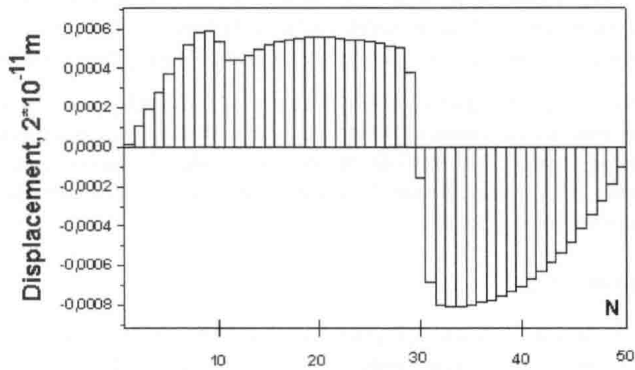


Figure 3. Displacement of 50 atoms of the excited nonlinear chain at the time of stabilization. *N* defines the atom number in the chain.

2.2. H–O–H molecule chain

We investigated the chain of H–O–H molecules shown in Figure 4. From two to eight molecules (6–24 atoms) were used. The equilibrium distances between H and O atoms inside the molecule are 0.96 Å, and the equilibrium distance between the molecules is 1 Å, which corresponds to ... Single impact was assumed, and the velocity of the first atom was varied from 100 to 1600 m/s, which corresponds to 10^{-5} – 10^{-2} eV of the exposed energy. Again, Morse potential was used.

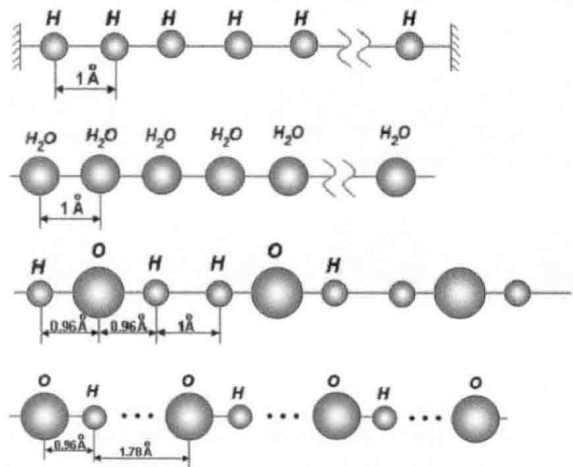


Figure 4. Atom chain of water consisting of hydrogen and oxygen atoms.