THEORETICAL ANALYSIS, DESIGN AND VIRTUAL TESTING OF BIOCOMPATIBILITY AND MECHANICAL PROPERTIES OF TITANIUM-BASED NANOMATERIALS

Rendicontazione

Informazioni relative al progetto

ViNaT

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Final Report Summary - VINAT (THEORETICAL ANALYSIS, DESIGN AND VIRTUAL TESTING OF BIOCOMPATIBILITY AND MECHANICAL PROPERTIES OF TITANIUM-BASED NANOMATERIALS)

Executive Summary:
The quality and reliability of medical implants determine the healing success, life quality and wellbeing of many people with artificial hips and knees, mechanical heart valves, dental implants. The requirements toward the materials for medical implants are quite challenging. Nanostructured metals are among the most promising materials which can satisfy these requirements. In order to make the development and optimization of nanostructured metallic biomaterials practically realizable, as well as to reduce unnecessary animal experimentation, reliable computational models for the virtual, numerical testing of these materials are necessary.
This project is devoted to the development of a complex of simulation tools for virtual testing and computational development of nanostructured and ultrafine grained titanium based materials for medical implants. In the framework of the project, a complex of computational models has been developed, allowing to analyze the mechanical behavior, strength and biocompatibility of ultrafine grained (UFG) titanium based materials for medical implants. The models, based on the methods of molecular and dislocation dynamics, crystal plasticity, polycrystal homogenization, computational micromechanics are employed here to analyze the mechanical properties and biocompatibility of Ti-based nanomaterials. The computational models were validated by comparison with experiments, and implemented as in newly developed software for evaluation of mechanical properties, structural evolution and biocompatibility of metallic materials for medical implants. Among other results, a new implant with low (2 mm) radius produced from ultrafine grained titanium as well as a novel processing route for fabrication of UFG-Ti with highly homogeneous structures were developed.
In the framework of the project, one international conference and two international workshops were organized by the consortium. 22 research papers were published in international journals. A special issue of international journal “Computational Materials Science” devoted to the project results has been published.

Project Context and Objectives:

Project context: Due to the rapid change in the age structure of the European population, an increasing number of people need their failed tissues to be replaced by artificial components such as artificial hips and knees, mechanical heart valves, dental implants, etc. Metallic materials (stainless steel, Co-Cr alloys and titanium and its alloys) are widely used for medical implants in trauma surgery, orthopaedic and oral medicine. Successful incorporation of these materials into clinical practice requires that they meet several critical criteria, namely, biocompatibility and mechanical strength. While the mechanical properties of materials can be increased by either alloying or secondary processing, for example rolling, drawing, etc., these operations often lead to an impairment of host response.
The most promising solution in this area is the development of nanostructured materials that can provide the required combination of high strength, biocompatibility and machinability. However, the development of new metallic nanomaterials for medical applications, fabrication technologies and micro/nanostructures require complex, very expensive and labour consuming experiments along with in vitro (cell culture) and in vivo (animal model) studies.
In order to make the development and optimization of nanostructured metallic biomaterials practically realizable, as well as to reduce unnecessary animal experimentation, reliable computational models for the virtual, numerical testing of these materials are necessary.
These models should provide computational tools for the analysis of the already available and the design of new, improved nanomaterials for medical applications, to allow both the predictions of their usability, mechanical properties, biocompatibility, and the optimization, microstructure design and development of new materials on the basis of virtual testing on the materials. The models to be developed should take into account the multiscale nature of the mechanical behaviour of these materials, interaction between macroscale loading and nano/microscale structures, and be validated by detailed experiments and by practical testing.

Objectives:
This project is devoted to the development of multiscale models for the theoretical analysis, virtual testing and optimization of three main groups of nanostructured titanium-based metallic materials: pure titanium, Ti-Nb alloy and superelastic/shape memory Ti-Ni alloy. The idea of the project is to develop and validate a series of computational models for these materials on the atomistic, crystal/dislocation and grain/texture/microstructure levels, to explore their biocompatibility and mechanical properties, and to analyse the effect of atomistic, nano and microscale structures on the properties of these materials.
Models based on the methods of molecular dynamics, dislocation dynamics, single crystal plasticity, polycrystal homogenization, discrete micromechanics are employed here to analyze the mechanical properties and biocompatibility of Ti-based nanomaterials.

The objective of the project is the development of multiscale models of mechanical behaviour and strength of nanostructured titanium and biocompatible nanostructured Ti-based alloys with superelasticity and shape-memory, taking into account the atomistic, dislocational and nano- and microscale structures and properties of the materials.
The project consists of 5 work packages, each of them had the following intermediate objectives::

WP1: Multiscale modeling of mechanical behavior and strength of biocompatible nanostructured titanium.
• Development and verification of multiscale models for the theoretical analysis, virtual testing and optimization of nanostructured titanium, taking into account the material structure and deformation

mechanisms on the atomistic, crystal/dislocation and grain/texture/microstructure levels; the modelling studies include quantum mechanical calculations of Ti metallic clusters and crystal structure, MD (molecular dynamics) calculations of deformation and structural transformations in nanostructured Ti; calculations of parameters of the diffusion processes at interfaces of nTi/fluids; analysis of grain boundary sliding and texture development in nanostructured Ti and of dissolution rate; identification of the operating mechanism triggering grain subdivision and development of a computer algorithm for a (micro)texture development modelingl in nTi with changing number of orientations.
• Development of optimal recommendations for the production of new nanostructured Ti materials, that would be applicable for manufacture of medical instruments and tools,
• Production and testing of a functional prototype of implantable medical appliance with higher load capacity than the implants produced nowadays from commercially pure Ti.

WP2: Multiscale modeling of biocompatible nanostructured shape memory and superelastic alloys.
• Development and verification of computational models for the theoretical analysis, virtual testing and optimization of nanostructured Ti-Ni and Ti-Nb-(Zr, Ta) SMA, taking into account their multiscale structures and deformation mechanisms at nano, micro, meso and macrolevels;
• Development of a computational models of martensitic phase transitions and plastic deformation by grain boundary sliding in nanostructured Ti-Ni alloys; Study of nucleation and development of structural and phase transformations in the crystallites of the alloys under severe plastic deformation; MD simulations of nanoindentation process in nanostructured NiTi materials.
• Development of a method for calculation of theoretical resource and crystallographic direction of the maximum recovery strain in Ti-Ni and Ti-Nb-(Zr, Ta) SMA single crystals and polycrystals and their dependencies on temperature, solid solution concentration, crystal lattice defects, crystallographic texture and conditions of strain inducing and recovery
• Experimental validation of the results of modeling of shape recovery characteristics in Ti-Ni and Ti-Nb-(Zr, Ta) SMA in various structure states including nanosubgrained and nanocrystalline ones

WP3. Modelling of biocompatibility of nanostructured titanium and Ti-alloys.
• MD calculations of the dissociation barriers for ion from a surface and grain boundaries into solution; Test and improvement of the atomistic potentials for the description of nanoindentation in biomaterials
• Establishing relationships between the specimen geometry, nano-grain size and microstructure of the near-surface layers (developing as a result of local vacancy supersaturation) of nanostructured Ti, TiNi and TiNb specimens, and the dissolution rate, surface oxide growth rate, the rate of Ca phosphate deposition, ion release rate and the concentration of Ca2+ and released metal ions (Ti, Ni, Nb) in the simulated body fluid (SBF);
• Modelling the chemical interdiffusion process along the grain boundaries (GB) of nanostructured Ti, TiNi and TiNb, with the emphasis on the difference in intrinsic diffusivities and atomic volumes of the diffusing species;
• Calculating internal stresses generated in the near-surface layer as a result of interdiffusion and their reciprocal effect on diffusion and dissolution;
• Assessing the biocompatibility of nanostructured Ti, NiTi and TiNb in various structure states using electrochemical tests.
• Investigation of the processing of nanostructured TiN PIRAC coatings on nano-Ti and TiNi and TiNb Ti alloys;

WP4: Modeling of nanoindentation and mechanisms of localized deformation of nanostructured biomaterials. The objective of this work package is to investigate the strength and mechanical properties of the multifunctional bioactive films and the substrate/coating systems to be used in implants to promote the formation of bone-like layer on the implant surface, prevent toxic ion release, and improve mechanical and tribological characteristics of implants. Understanding the fracture mechanisms during indentation, scratching and impact testing is critical for understanding how the film/substrate system will perform in service, and determination of reserves o9f their improvement. The objectives include:
• Modelling the mechanical behavior of heterogeneous nanostructured protective and bioactive coating on Ti-based nanostructured materials under nanoindentation, including molecular dynamics (MD) simulations of nanoindentation process in Ti and NiTi alloys using accurate classical potentials for interatomic interactions,
• Determination of load-displacement curves for various NixTi1-x samples, stress-strain distributions and stress evolution in nanoindentation; analysis of the influence of grooves, grain boundaries and other crystal structure defects on the materials' behaviour under nanoindentation; analysis of the deformation localization in biocompatible NiTi materials.

WP5: Management and coordination. The main objective is to establish and ensure efficient organization of the project and collaboration between partners during all the project time, which includes: Management and coordination. Administration of financial transmissions; Organization of regular project meetings and discussions; Preparation of Consortium and Coordination agreements; Preparation of Software Co-ownership Agreement; Coordination and interaction with the sister project in Russia; Monitoring the compliance by beneficiaries with their contractual obligations.

Project Results:
The results include a complex of advanced computational models, allowing the analyze the mechanical behavior and biocompatibility of nanostructured metallic materials at the atomistic, dislocation and microstructural scales, the modular software complex for virtual testing of nanostructured materials for medical applications, a number of technologies of produce the nanostructured materials with required, improved structures, and advanced testing procedures for the model validations.

1) COMPUTATIONAL MODEL COMPLEX: The model complex include the molecular dynamics model of formation and structure formation of nanostructured titanium and atomistic determination of elastic properties of nTi, FE crystal plasticity model of deformation of polycrystalline nano-Ti model; FE micromechanical deformation of nanostructured and ultrafine grained nanotitanium, used for the analysis of dislocation density evolution in the material, effect of grain size and non-equilibrium grain boundary on the mechanical behaviour of nano-Ti, and experimental validation of these models; dislocation evolution analysis of the deformation of nano-Ti, identification of the operating dislocation mechanisms triggering the grain subdivision and the development of a grain subdivision model in nano-Ti; large scale molecular dynamics simulations of diffusion processes on interfaces of nTi and TiNi with fluids, and of the nanoindentation process of a bimetallic nickel-titanium crystal which allowed to identify the different deformation regimes depending on the geometry of the indenter.
This “virtual laboratory”, a series of theoretical models which allow analysis the mechanical and biological response of nanostructured materials, and allows improvement and design these materials, would greatly

accelerate the process of development and optimization of new biocompatible materials. With the developed models, the analysis of interrelationships between the production technology, nano- and microstructure and service properties can be carried out what would allow to find the reserves of improvement of production technologies, improve these technologies and enhance materials properties. This will lead to the quick efficient virtual testing and development of new biocompatible materials for medical implants, and allow the quick, efficient and reliable development of the biocompatible nanometallic materials for medical applications, without in vivo tests on animals or humans. Among many elements of this series of models, one should also mention the new crystal plasticity (CP) model of nanometals, developed and implemented in the FE code ABAQUS. The model allows to simulate tensile deformation and drawing process and to estimate the effective properties and mechanical behaviour of polycrystalline nano-Ti taking into account their microscale and nanoscale structures.

The computational models have been published in around 20 papers in international journals, presented at 6 international conferences, in different other media, like TV, press-releases, 3 special international conferences were organized in the framework of the project, etc. Further publications are under way, and more presentations are planned.

2) SOFTWARE COMPLEX: Software complex for multiscale virtual testing of nanoTi and Ti-alloys, including 8 modules, in particular, nanoindentation database of MD simulations of nanoindentation in Titanium-based alloys and of various mechanisms of diffusion, and localized deformations on atomistic scale, estimation of “Taylor factor” for a given texture of Titanium and yield stress of ultrafine grained (UFG) titanium with non-equilibrium grain boundaries, modelling of kinetics of the disintegration by formation of pores as a result of vacancy diffusion along grain boundaries of different nanostructured materials and different conditions of the experiment, such as grain size, temperature, evaluation of the shape recovery parameters, analyze of crystal behavior under complex mechanical loading at atomic scale, etc.

The software makes it possible for industrial users to get estimations of service properties of nanomaterials in development, thus, enabling the companies the development of new materials and comparison of available materials for medical applications. The software can be used by the industry, by companies working in the area of development of advanced nanostructured biocompatible materials for medical applications. The program complex will be an effective tool for choosing the specific composition and processing parameters of nanostructured biocompatible alloys for various applications. The potential users are allowed to acquire the programs to evaluate and predict the service properties of nanostructured biocompatible metallic materials, and thus, choose and design appropriate materials for the medical applications. This would simplify and speed up the development and use of nanostructured materials for implant and other medical applications.
With increase of fabrication capacities of nanostructured biocompatible Ti based alloys and accumulation of experimental results regarding mechanical behavior and biocompatibility of developed alloys, the models and the program complex will be updated and optimized to fit the needs of developing market. Ultimately, the development of strong, reliable and biocompatible materials to be used in medical applications should lead to new possibilities in trauma surgery, orthopaedic and oral medicine. Ultimately, the bone illnesses, dental problems, traumas can be healed at the fully new level, as soon as the new, reliable, biocompatible materials are available. Many people, who suffer from the bone or dental diseases

now, can be brought back to active life.
The faster and more efficient development of new materials for medical applications will not only help to save the health and even life of thousands of people, but create an important, quick developing industry branch.
The software is available online. The procedure of maintaining, exploitation and marketing of the software is regulated by the software agreement and the Memorandum of Understanding about Further Collaboration, signed by the partners. The exploitation includes: maintaining and support; regular improvement, upgrading and enhancement on the basis of further modelling work; presentation to implant materal developeds (Rontis, Johnson and Johnson); presentations at special conferences and meetings; collaboration with the software companies including QuantumWise (Danish company), Quantech (Spanish software company), etc.

3) NEW NANOTITANIUM BASED IMPLANTS WITH SMALL RADIUS (2.0 mm) can withstand loads similar to those carried by implants of conventional design with a diameter of 3.5 mm made from coarse-grained Ti.. The implants are made from pure Ti and, therefore, does not contain any toxic alloying elements (like V) and elements classified as allergens (like Ni, Co, or Cr).
Prototype testing: Prototype of an implant with diameter of 2.0 mm (Vinat) was applied to a 18 year old patient (by stomato-surgeon MUDr. M. Brückner), who was after long orthodontic treatment, and who agreed to the application of this type of implant. The patient did not have basis of his own natural teeth in the areas 12 and 22. After examination and after investigation of several radiographs the dental surgeon decided that in the area 22 (the second tooth on top left) did not have a suitable bone and that he would not implant into this locality an implant with the diameter of 2.4 mm due to lack of transverse dimensions of the bone. The results of the control (after one and 2 months) were positive. Another potential application of this implant material is to prevent bone breakage for osteoporosis risk groups.
After a six-month monitoring of the Vinat implant in the patient's mouth it can be stated that the implant withstands normal physiological loads without any problems and the process of osseo-integration runs in the manner that is usual for the implants Nanoimplant with diameter of 2.4 mm. During the period of monitoring another Vinat implant was applied, which was regularly checked by the dentist who applied it – with the same result.
Development of nTi, the parameters of which would be “tailor made” to the given application is also worth consideration. The present development is oriented mostly on the requirements of implantology. For example development of nTi for its use at manufacture of the spherical attachment must combine such parameters as strength, hardness and resistance to abrasion. The manufacturers then would not have to use different technologies of surface treatment of spherical attachments and matrices.

4) GRADED COATINGS WITH EXCELLENT ADHESION ARE USABLE ON NANOMETALS: PIRAC Coatings (with excellent adhesion) usability of nanotitanium: it is shown that TiN based Reactive Diffusion coatings can be obtained on nano-Ti and nano-TiNi with retention of nanoscale structure via PIRAC nitriding treatments at relatively low temperatures. In PIRAC (Powder Immersion Reaction Assisted Coating) coatings graduate change of composition results in graduate change of properties, such as microhardness, and thus in excellent adhesion of the coating to the substrate.
The Pirac coatings applicability on nanometals opens new perspectives in the development of new medical implants with very good adhesion of coatings and extraordinary properties of substrate (nanomaterials).

Advanced technologies of fabrication of nanomaterials with enhanced structures: Novel processing route for fabrication of nano-Ti with a very homogeneous microstructure consisting of equiaxed grains and improved properties was developed.
The novel processing route for fabrication of nTi includes ECAP-C processing at 200oC followed by drawing at 200oC into cylindrical rod. TEM analysis showed that this processing route leads to formation of a very homogeneous microstructure consisting of equiaxed grains
The technology should be further investigated and optimized using the developed models and software. After that, the necessary patents applications are planned (by the consortium member NanoMet).The technology will be presented to the manufacturers and employed to the fabrication of bulk ultrafine grained titanium specimens with homogeneous structure and high strength and toughness.

Potential Impact:
The potential impact of these results include the following directions:

A) COMPLEX OF ADVANCED MULTISCALE MODELS for the analysis of the mechanical behavior and biocompatibility of nanostructured metallic materials: Efficient, mechanism based development and improvement of new biocompatible materials for medical implants. The development of the new, fully biocompatible and high strength materials requires a lot of investigations, and would be prohibitively expensive and labour consuming if all these investigations are carried only experimentally. Advanced multiscale models for the predictive simulation and virtual testing of the mechanical behavior and biocompatibility of nanostructured metallic materials will allow the quick, efficient and reliable development of the biocompatible nanometallic materials, that will not require in vivo tests on animals or humans.
The development of “virtual laboratory”, a series of theoretical models which allow analysis the mechanical and biological response of nanostructured materials, and allows improvement and design these materials, would greatly accelerate the process of development and optimization of new biocompatible materials. For the quick, efficient and reliable development of the biocompatible nanometallic materials, theoretical, test based methods to study and model the biocompatible metallic materials for medical applications are needed that will not require in vivo tests on animals or humans.
With the developed models, the analysis of interrelationships between the production technology, nano- and microstructure and service properties can be carried out what would allow to find the reserves of improvement of production technologies, improve these technologies and enhance materials properties. This will lead to the quick efficient virtual testing and development of new biocompatible materials for medical implants.

B) MODULAR SOFTWARE COMPLEX for virtual testing of nanostructured materials for medical applications: The complex of computational programs can be used by the industry, by companies working in the area of development of advanced nanostructured biocompatible materials for medical applications. The program complex will be an effective tool for choosing the specific composition and processing parameters of nanostructured biocompatible alloys for various applications. The program will make it possible for industrial users to get estimations of output and service properties of nanomaterials in development, thus, enabling the companies the development of new materials and comparison of available materials for medical applications. The potential users will be able to acquire the programs to evaluate and predict the service properties of nanostructured biocompatible metallic materials, and thus, choose and design appropriate materials for the medical applications. This would simplify and speed up the

development and use of nanostructured materials for implant and other medical applications.
With increase of fabrication capacities of nanostructured biocompatible Ti based alloys and accumulation of experimental results regarding mechanical behavior and biocompatibility of developed alloys, the models and the program complex will be updated and optimized to fit the needs of developing market.
Ultimately, the development of strong, reliable and biocompatible materials to be used in medical applications should lead to new possibilities in trauma surgery, orthopaedic and oral medicine. Ultimately, the bone illnesses, dental problems, traumas can be healed at the fully new level, as soon as the new, reliable, biocompatible materials are available. Many people, who suffer from the bone or dental diseases now, can be brought back to active life.
The faster and more efficient development of new materials for medical applications will not only help to save the health and even life of thousands of people, but create an important, quick developing industry branch.
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C) Advanced TECHNOLOGIES OF FABRICATION OF NANOMATERIALS WITH ENHANCED STRUCTURES and the new small radius high strength implants: The investigations, developed model and simulations made it possible to develop several new technologies which can be used to fabricate highly strong and reliable materials for medical implants. New processing technology for production of highly homogeneous UFG metals of equiaxed grains allows to fabricate the very strong titanium based materials.
The newly developed and tested small radius implant (with the radium 2 mm) can sustain the same load as the old 3.5 mm radius implants, thus, making the surgery easier and usable even in difficult implantation cases.
The small radius implants can be used to reduce surgery effects, minimize patients pain, and are for instance usable as implants for patients with low volume of bones and other problems limiting the

application of traditional implants. Thus, these technologies can allow to improve healings of patients with bone and gums problems, thus, playing an important role in dentistry and implantology.

2. Main dissemination activities:
- Series of international conferences/workshops with broad participation from world leading universities, industry, many countries, organized by the project team: International Conference on Computational modelling of nanostructured materials, September 4-6, 2013, Frankfurt am Main, Germany, International Workshops on Modeling and development of nanostructured materials for biomedical applications, February 5-7, 2014, Madrid, Spain, International Workshops on Nanostructured titanium based alloys for medical applications, January 21-23, 2013, Ein Gedi, Israel,

- Special isue of the international journal ”Computational Materials Science”, edited by the project coordinators and presenting the collection of papers and results obtained in this project (Computational Materials Science, Special Issue “VirtualNanotitanium” ,Vol. 76, August 2013)

- Press-releases and publications in popular press (Online Journal Nanotech.com DTU webpage in Danish, MISIS webpage, etc.)

- Presentations by project participants at international scientific meetings (both meetings organized by the consortium members and others), totally 19 presentations

- Direct contact with industry, presentations and discussions with industry representatives

Main dissemination activities:
1) Publications in leading international journals with high impact factor: 20 papers åublished, 7 more submitted or in preparation
2) Special issue of the international journal ”Computational Materials Science”, edited by the project coordinators and presenting the results obtained in this project (Computational Materials Science, Special Issue “VirtualNanotitanium” ,Vol. 76, August 2013)
3) International Conference on Computational modelling of nanostructured materials, September 4-6, 2013, Frankfurt am Main, Germany, organized by the project conossortium, with broad participation from world leading universities and industry,
4) Two international workshops with broad participation from world leading universities and industry, International Workshops on Modeling and development of nanostructured materials for biomedical applications, February 5-7, 2014, Madrid, Spain, International Workshops on Nanostructured titanium based alloys for medical applications, January 21-23, 2013, Ein Gedi, Israel,
5) Press-releases and publications in popular press (Online Journal Nanotech.com DTU webpage in Danish, MISIS webpage, etc.); 4 publications in popular press and press-releases
6) Presentations by project participants at international scientific meetings (both meetings organized by the consortium members and others), totally 19 presentations, 7 international conferences,
7) Direct contact with industry (Johnson and Johnson, Rontis), presentatioins and discussions with industry representatives

EXPLOITATION:
The Dissemination and Exploitation activity has been planned in the following directions: Awareness and effective communication of the project activities; communication of research findings; Establish and reinforce a wide network of potential contacts and customers; Building reputation with industries and potential partners; Definition and execution of activities such as workshops, conferences, journal publications and internet exposure; Evaluation of achieved results through appropriate feedback mechanism; Analysis of exploitatioon and business opportunities.
During the project time, a lot of potentially exploitable results were developed, which can be transformed into products and brought to the market in due time. Among them, one can list the complex of theoretical and computational models describing the mechanical properties and biocompatibility of nanostructured Ti-based materials, software complex (concept and some modules of the software for multiscale virtual testing of nanoTi and Ti-alloys), developed nanotitanium based dental implants with smaller diameter (less than 2 mm), novel processing routes for improving nano-Ti.
For the optimal exploitation and dissemination of these results, the special steps and activities have been implemented, including the series of special conferences/workshops, special journal, pubklications, presentations, press-releases, etc. Special analysis allowed to identify most important and promising results, as well as potential users (inside and also outside of the consortium). Several companies were identified, which have been approached with view on further collaboration for the further development, exploitation, and bringing the results to the market; while the nTi based implants will be further developed inside the consortium (by Timplant, in collaboration with USATU, IMDEA and others), several results will need further external collaboration (like software companies, to join further development of software, and medical device companies, to use Ti-based materials). Special efforts will be done for the continuation of the collaboration inside consortium, acquiring additional funding and continuation of work, to ensure practical applicability and successful exploitation of the project results.
With view on the exploitation and commercialization of the new nTi based implants with lower radius (2.0 mm), the partner Timplant established the collaboration with dental clinics in Ostrava (MUDr. M. Brückner) for further testing of the small radius implants. Necessary steps for certification and licensing will be implemented. The negotiations with dentists in clinics (for initial evaluation) will be started. It is expected that small radius implants will play role of a niche product, for patients with reduced bone volumes in some regions. After the initial testing phase, the implants will be presented to dentist groups in Czech Republics and Germany.
The ideas and concepts of the developed computational models have been published in around 20 papers in international journals, presented at 6 international conferences, in different other media, like TV, press-releases, 3 special international conferences were organized in the framework of the project, etc. Further publications are under way, and more presentations are planned. The models will be tested on different materials, as well as generalised to other medical materials (magnesium, iron, etc.). The models will be presented to software developers and users, as well as other research groups working on this subject.
The modular software complex for virtual testing of nanostructured materials for medical applications is available online. The procedure of maintaining, exploitation and marketing of the software is regulated by the software agreement and the Memorandum of Understanding about Further Collaboration, signed by the partners. The exploitation includes: maintaining and support; regular improvement, upgrading and enhancement on the basis of further modelling work; presentation to implant materal developers (Rontis, Johnson and Johnson); presentations at special conferences and meetings; collaboration with the software companies including QuantumWise (Danish company), Quantech (Spanish software company),

etc.
The further exploitation plan includes: presentations of the obtained results, dissemination and commercial negotiations with the potential users (identified in the market analysis carried out in the project), in software exploitation, QuantumWise, Quantech, others; dental clinics as small radius implant users); preparation of detailed business plan between the consortium members and external industries; identification of possible reserves of improvement and further collaboration with external industries to bringing the foregrounds on the market; further presentations of results on conferences, special meetings and direct contacts with potential users; further collaboration of the project consortium for the generalization, improvement, development, upgrading and maintaining the foregrounds; definition of the important tasks for the further development of the model complex, software and medical implants.

List of Websites:
Address of the project public website:
http://www.risoecampus.dtu.dk/Research/sustainable_energy/new_energy_technologies/projects/AFM_vinat.aspx

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