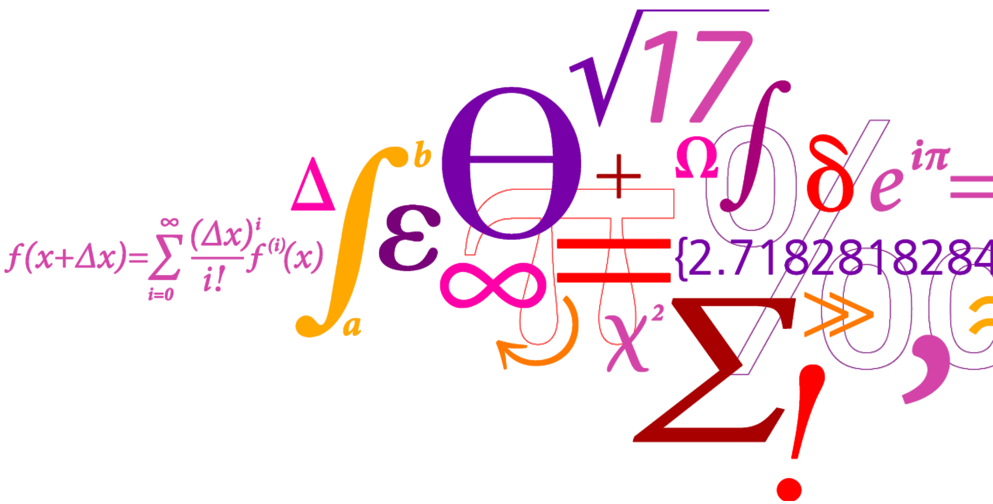
EU FP7 PROJECT

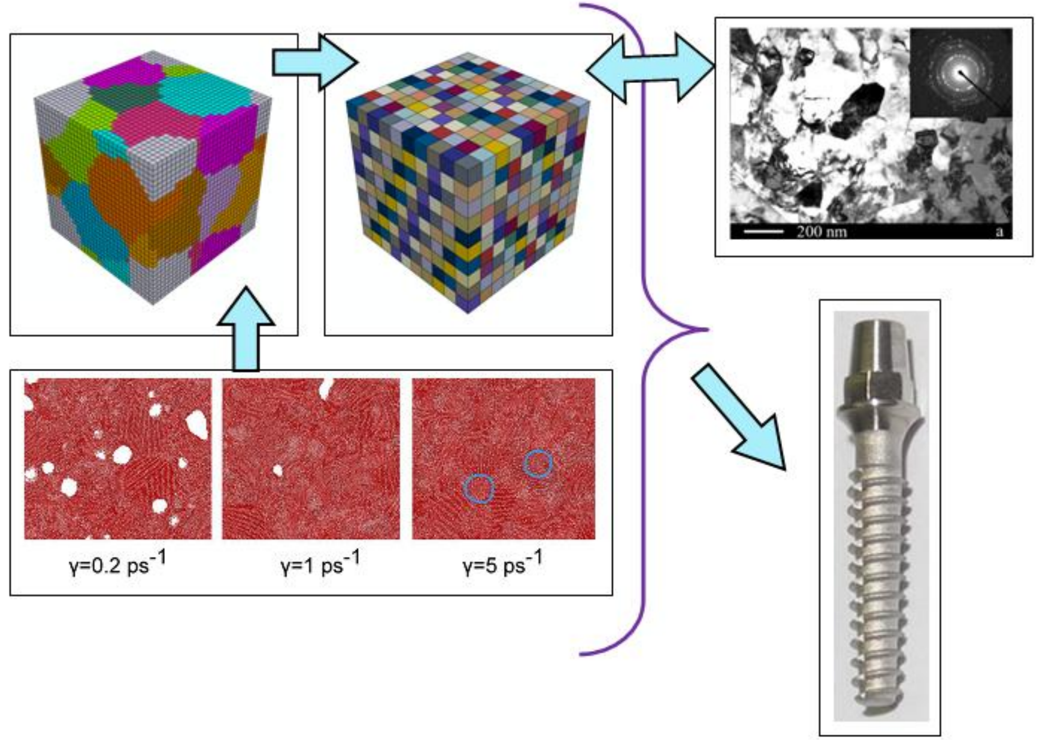
VIRTUAL NANOTITANIUM (VINAT)

SEVENTH FRAMEWORK PROGRAMME

Theoretical analysis, design and virtual testing of biocompatibility and mechanical properties of titanium-based nanomaterials

THEME: NMP.2011.1.4-5 Multiscale Modelling as a Tool for Virtual Nanotechnology Experimentation (Collaborative project . Coordinated call with Russia).





The objective of this project is to develop **computational multiscale models for virtual testing** and design of biocompatible, Ti-based materials for implants and other medical applications

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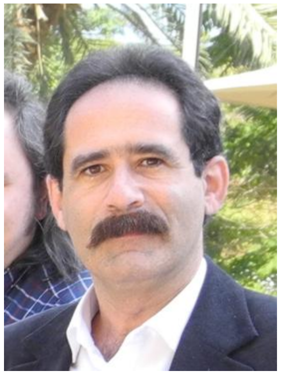

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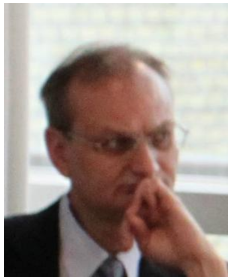

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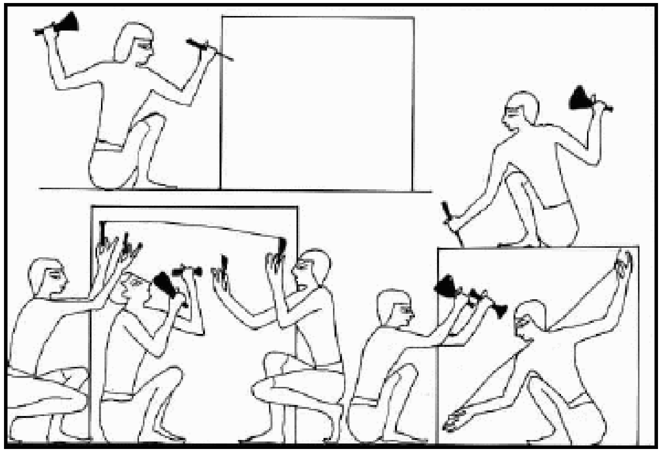
WORK PACKAGES

1. Multiscale modeling (MM) of mechanical behavior and strength of **biocompatible nanostructured titanium**
2. Modelling of biocompatible **nanostructured SMA and superelastic alloys**
3. Modeling of **biocompatibility** of nanostructured titanium and Ti-alloys
4. Modeling of **nanoindentation** and mechanisms of **localized deformation** of nanostructured biomaterials



WP1. MULTISCALE MODELLING OF NANOSTRUCTURED TITANIUM

WP1: Multiscale modelling of nTi

T1.1. Atomistic modelling of nTi (FIAS)

T1.2. Crystal/dislocation level modelling (IMDEA)

T1.3. Texture evolution (KUL)

T1.4. Grain boundary sliding (Techn)

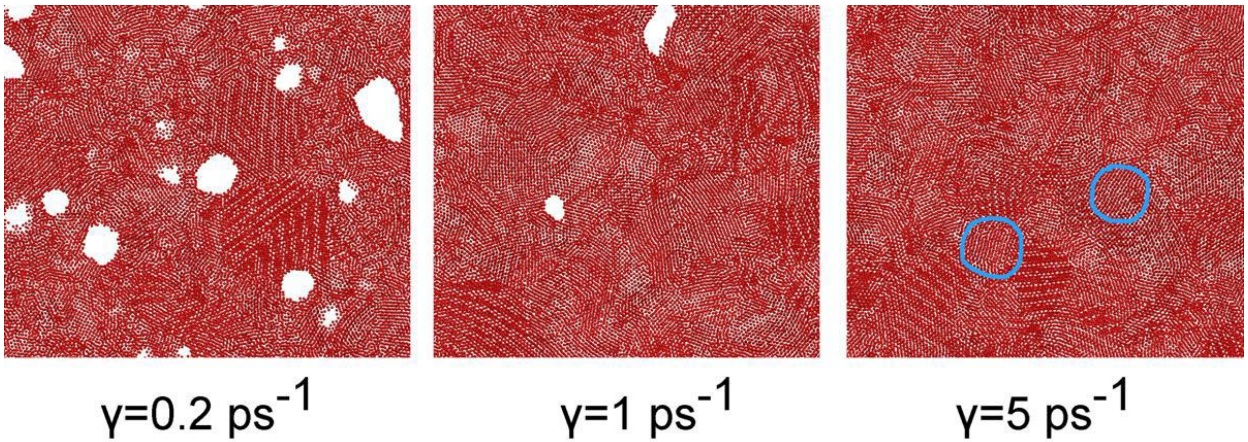
T1.5. Micromechanics of nTi (DTU)

T1.6. Experimental validation

T1.7. Severe plastic deformation (USATU)

T1.8.TEM, SEM (USATU, NM)

Task 1.1. Atomistic modeling of deformation of nanotitanium (FIAS GU)



Structure of the solid-state nano-Ti samples obtained at different values of the coupling parameter between the system and the thermostat. Strong coupling leads to the formation of cavities, while slower cooling rate allows producing large sizes of monocrystalline grains

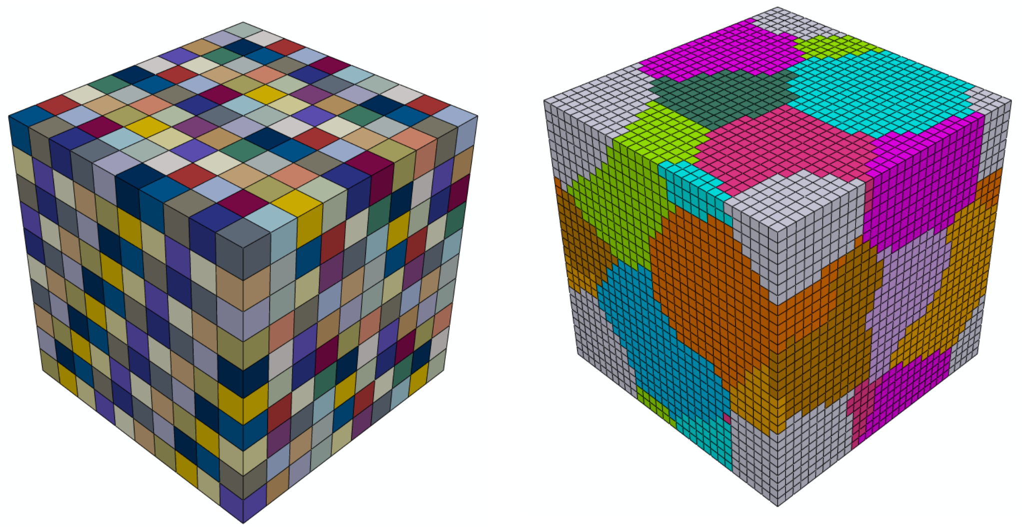
Results:

- ❑development of a molecular dynamics model of the structure formation of nanostructured titanium
- ❑atomistic determination of elastic properties of nTi.

- ○The first-principles calculations using density functional theory (DFT) within a plane-wave pseudopotential approach, implemented in ABINIT package

- ○Molecular dynamics simulations of nanocrystalline Ti using computer package MBN Explorer. The classical force fields describing the many-body interactions of Ti atoms are based on the Finnis-Sinclair-type of potential

Task 1.2. Modelling Crystal/Dislocation Level (IMDEA)



Representative volume elements of polycrystalline Ti. (a) Voxel model with 1000 cubic finite elements in which each one stands for a single crystal. (b) Realistic RVE containing 100 crystals discretized with 64000 cubic finite elements.

- **Crystal plasticity** (CP) model of nTi developed and implemented in the FE code ABAQUS using a UMAT subroutine.
- Effective properties of polycrystalline nano-Ti determined.

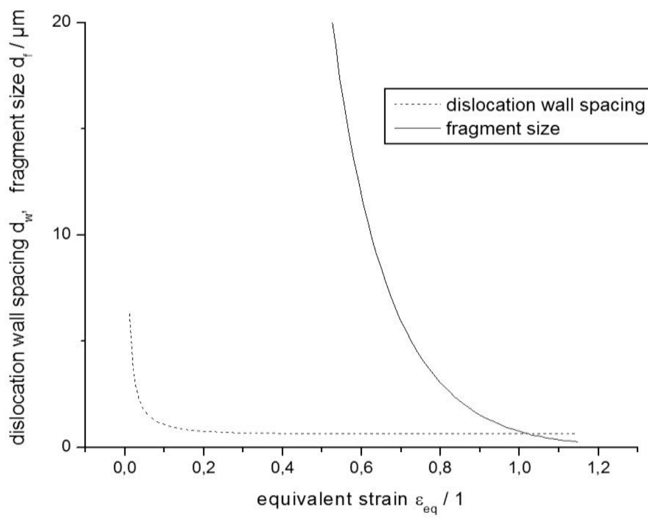
Two different representation of the microstructure were used: a voxel-based model and a finite element discretization with cubic elements but each crystal is represented with many elements. In either RVE of the polycrystal, the orientation of each grain was determined from the input orientation distribution function (ODF) which describes the initial texture using a Monte Carlo lottery.

- **Simulation of tensile deformation and drawing process.**

Results:

- ❑ development of a crystal plasticity, finite element model of deformation of polycrystalline nano-Ti model, its validation and simulation of the drawing process.

Task 1.3. Microstructure Evolution: defect storage, grain subdivision and texture evolution model for cold deformation processing (KU Leuven)



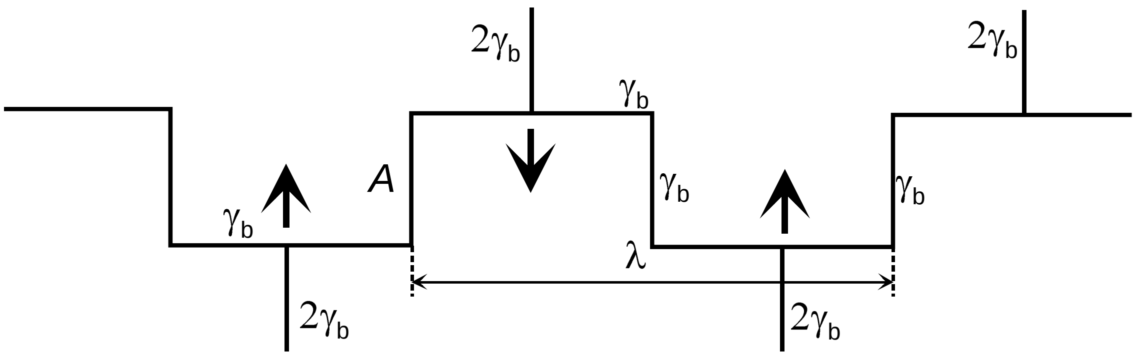
Dislocation wall spacing and fragment vs. equivalent strain.

- ❑ Balance equations for the evolution of dislocation and disclination densities with accumulated plastic strain derived. They include physically based terms for the generation, storage and annihilation rates of the respective lattice defects..
- ❑ Substructure evolution calculated separately for each grain orientation and thus set of slip activities.

Results:

- ❑ dislocation evolution analysis in the grains of nano-Ti, identification of the operating dislocation mechanisms triggering the grain subdivision and the development of a grain subdivision model in nano-Ti.

Task 1.4. Modeling of plastic deformation by grain boundary sliding (Technion)



Model of anisotropic undulated GB which straightens during sliding by the GB migration mechanism. The directions of GB migration are shown by the arrows.

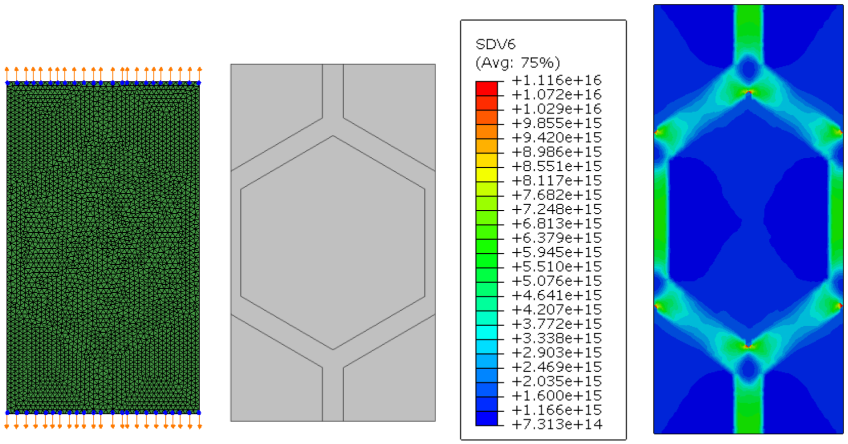
- Simple 'toy' models illustrating the contributions of accelerated diffusion along the triple junction, of nucleation of Shockley partials at the GBs, and of GB migration to the kinetics of GB sliding in nanocrystalline material. developed,

Results:

- ❑ development of a theoretical model of the grain boundary sliding taking into account the GB migration, effect of trip junctions and diffusion coefficient along the triple junctions, which allows to capture grain boundary evolution and formation of macroscopic shear bands.

Task 1.5. Micromechanical modeling of deformation and yield strength of nanostructured titanium (DTU)

DTU



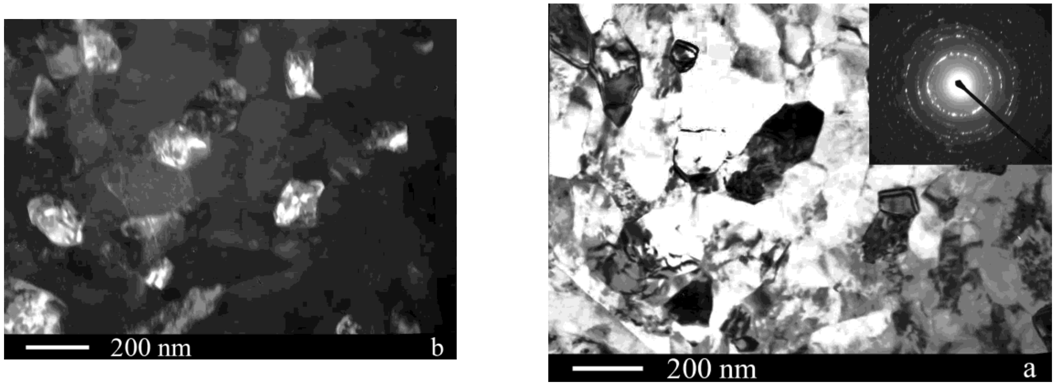
Geometrical model of nanostructured Ti with grain and grain boundary phase, and DD distribution

- ABAQUS Subroutine VUMAT was developed, to calculate the dislocation density evolution in grain and GB phases.
- dislocation density increases much more intensively in GBs than that in grains with deformation increasing.
- obtained the relationship between the yield stress of nanostructured metallic material and the excess free volume in grain boundaries

Results:

- development of a computational model of deformation of nanostructured and ultrafine grained nanotitanium, which allows to predict correctly the non-homogeneous dislocation density evolution in the material, as well as the effect of grain size and non-equilibrium grain boundary on the mechanical behaviour of nano-Ti.

Task 1.6. Experimental validation (IMDEA)



Microstructure of pure Ti after ECAP-C processing for 6 passes and drawing: a) longitudinal section, b) transversal section [15].

Results:

- ❑ development of a novel processing route for fabrication of nano-Ti, its microstructural and mechanical characterization

- ❑ novel processing route for fabrication of nano-Ti developed (subjected to ECAP-C processing at 200oC followed by drawing at 200oC into cylindrical rod
- ❑ TEM analysis of the microstructure shown that this processing route leads to formation of a very homogeneous microstructure consisting of equiaxed grains having the average size of ~150 nm
- ❑ Strength of nano-Ti increases with increasing strain rate and decreases with increasing temperature

Task 1.6. Experimental validation (TIMPLANT)

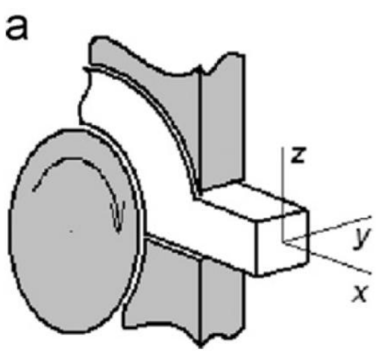
Scheme of implant from nanostructured Ti, (d) Prototype model of 2.2 mm-implant

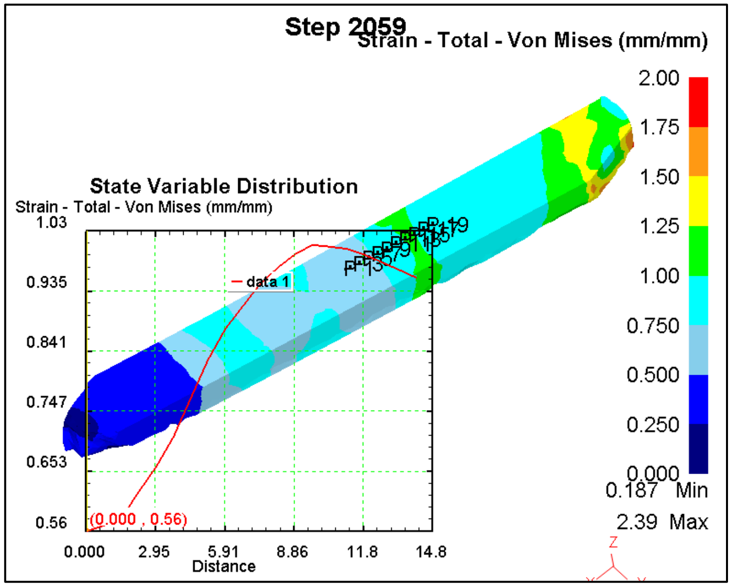
- ❑ developed implant with a diameter of 2.4 mm can withstand loads similar to those carried by implants of conventional design with a diameter of 3.5 mm made from coarse-grained Ti.
- ❑ The implant is made from pure Ti and, therefore, it does not contain any toxic alloying elements (like V) and elements classidfied as allergens (like Ni, Co, or Cr).

Results:

- ❑ fabrication of first prototype of dental implant.

Task 1.7. Modeling of deformation processes, evolution of microstructure, texture and dislocation structure under severe plastic deformation (USATU).





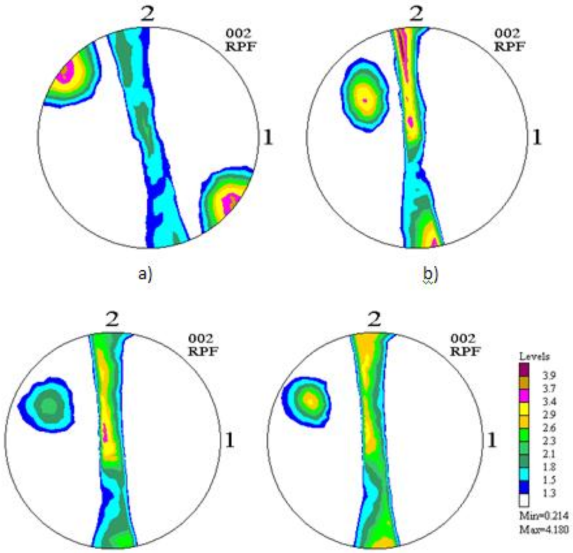
Distribution of shear strain in a Ti billet after 4 ECAP-C passes.

Results:

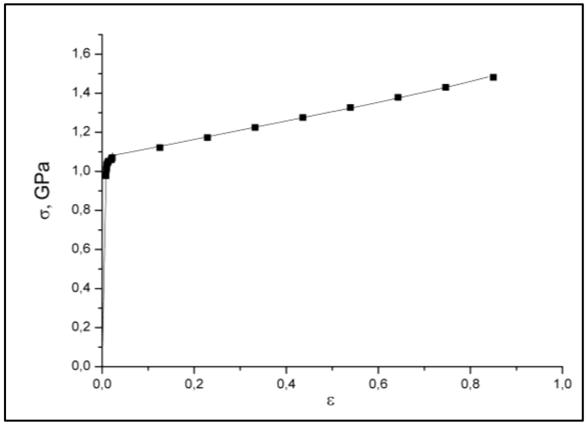
- ❑ multi-scale model of microstructure (grain size, dislocation density, vacancy concentration) in pure Ti after ECAP-C processing

- ❑ On the macro-level, a FEM-model for ECAP-C processing of Ti was developed
- ❑ Meso-level, CP model (visco-plastic self-consistent model) used to calculate texture evolution in TI during ECAP-C processing as well as to simulate deformation and slip system activity and output textures.
- ❑ Micro-level: disclination criterion for grain subdivision developed taking into consideration the grain refinement process

Task 1.8. Experimental validation (Nanomet, USATU).



Experimental pole figures (0001) in plane XZ after different number of ECAP-C passes: a) 1 pass, b) 2 passes, c) 4 passes, d) 8 passes.



True stress vs. true strain during tensile testing of nano-Ti produced via: a) ECAP-C for 6 passes (Line - modeling results, Points - experimental results).

- ❑ theoretical stress-strain curves derived from modeling of mechanical behavior of nano-Ti were validated against experimental results from tensile testing of this material
- ❑ experimental texture measurements using X-Ray technique showed that the crystallographic texture developed in Ti during ECAP-C processing is well predicted by the meso-level CP model

Results:

- ❑ Experimental results confirm the simulations

RELATIONSHIPS BETWEEN TASKS

DTU

T1.1. MD determination of elastic properties of nTi (FIAS)

T1.2. Crystal Plasticity model of deformation (IMDEA)

T1.4. Grain boundary sliding model of deformation (Technion)

T1.5. Micromechanical (composite) model of nTi and GB properties effect (DTU)

T1.6. Experimental validation (IMDEA) and implant development (Timplant)

Multiscale Model of Deformation and Strength of nT

T1.1. Atomistic model of structure formation (FIAS)

T1.3. Dislocation analysis of grain subdivision and structure evolution (KUL)

T1.7. Multiscale model of microstructure evolution under ECAP (USATU)

T1.8. Experimental validation/ ECAP (USATU)

Multiscale Model of Microstructure Formation in nTi

WP2. MULTISCALE MODELLING OF NANOSTRUCTURED NITINOL

WP2: Multiscale modelling of nSMA.

T2.1. Grain boundary sliding in SMA (Techn)

T2.2 Micromechanics & strength of SMA (DTU)

T2.3. Experim validation (Characterization) (IMDEA)

T2.4. Crystal lattice model of SMA (MISIS)

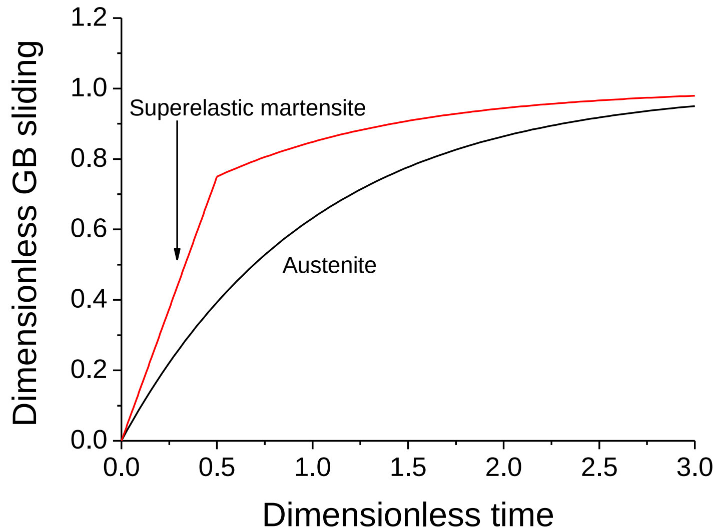
T2.5. Martensitic deformation (MISIS)

T2.6.Microstructure evolution (USATU)

T2.7. MD and continuum modelling (ISPMS)

T2.8. Validation-Thermomechanical tests (MISIS)

Task 2.1. Modelling of plastic deformation by grain boundary sliding in nanostructured Ti-Ni alloys (Technion)



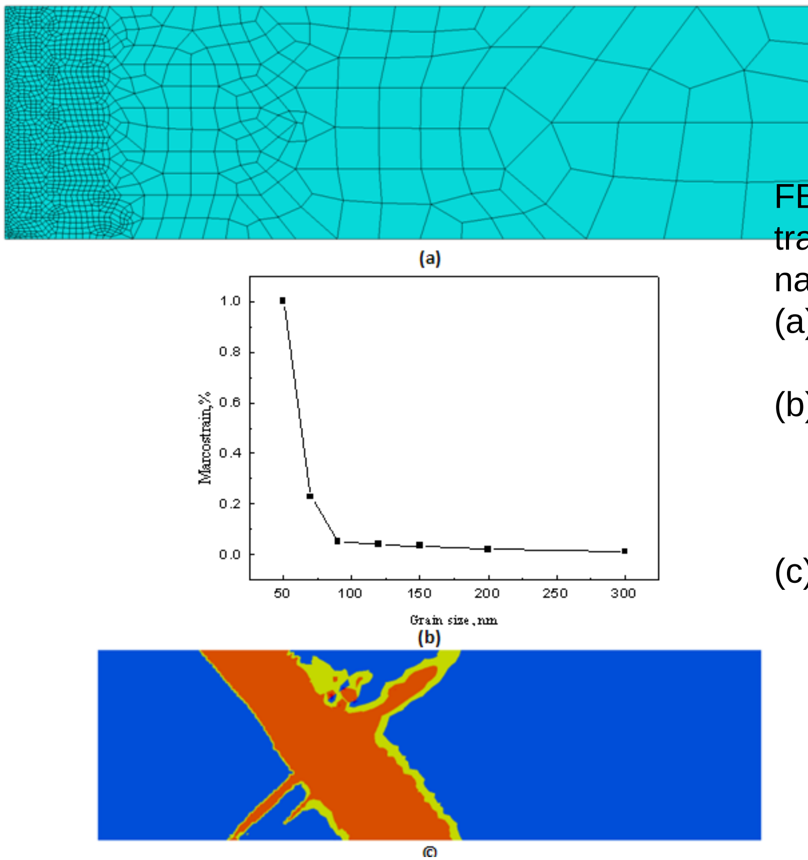
Acceleration of GB sliding in superelastic Nitinol

- ❑ GB sliding model for superelastic NiTi with deformation mechanisms including grain boundary diffusion, grain boundary sliding and B2-to-B19 martensitic transformation.
- ❑ superelastic contribution to the grain shape accommodation during GB sliding, a unique mechanism characteristic for the NiTi alloy, can significantly increase the contribution of GB sliding to the overall plastic strain.

Results:

- ❑ generalization of the grain boundary sliding model of plastic deformation to nanocrystalline nitinol

Task 2.2. Micromechanical modeling of deformation of nanostructured alloys with shape-memory effect (DTU)



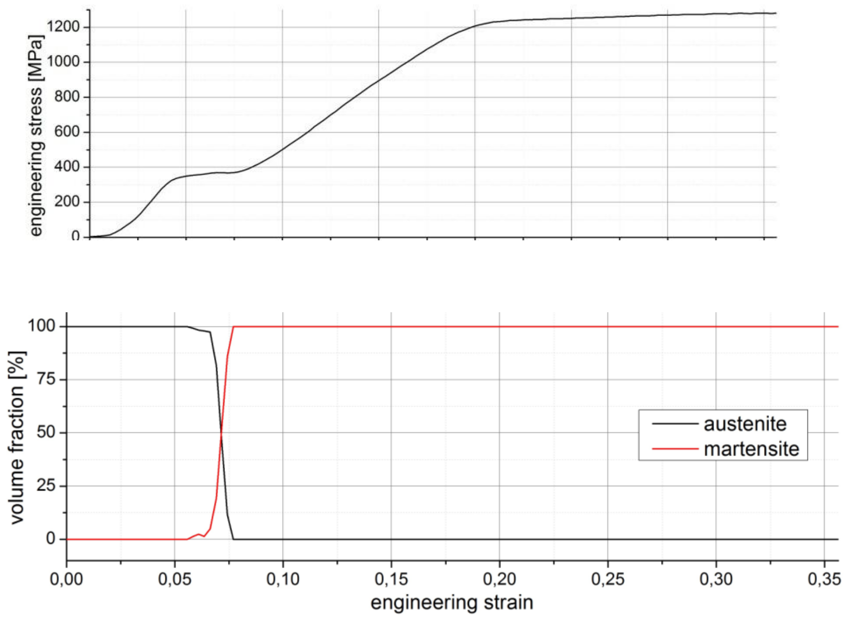
FE model of martensitic transformation in nanoNiTi:

(a) Graded grain distribution,
(b) Effect of grain size on the strain at which the martensite content reaches 5%
(c) Martensite distributions evolution at applied strain 0.4%

- ❑Computational model of martensitic phase transformations in nanonitinol based on thermodynamic theory
- ❑FE simulations of phase transformations and structure evolution in nanonitinol
- ❑Volume content of martensitic phase decreases drastically with reducing the grain size. When the grain size <50…80 nm, phase transformations are suppressed.
- ❑Graded distributions of grain sizes are studied

Results: development of a computational thermodynamics based model of martensitic phase transitions in nanonitinol, which includes effects of grain size, thermodynamical and mechanical properties

Task 2.2. Experimental validation of the modeling results. Different production methods (IMDEA, Technion)

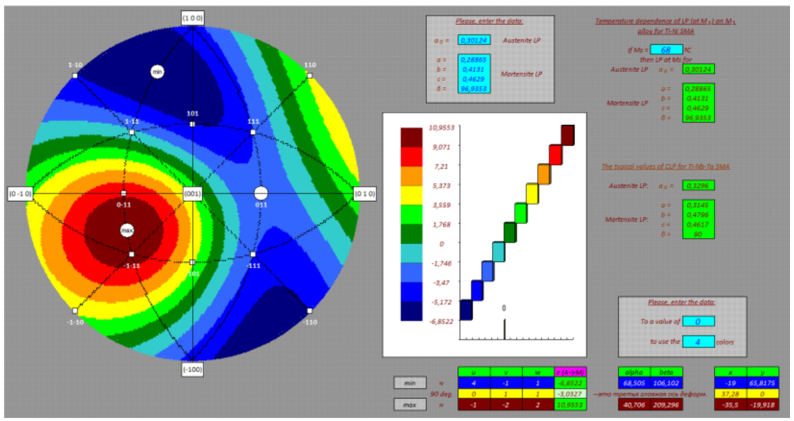


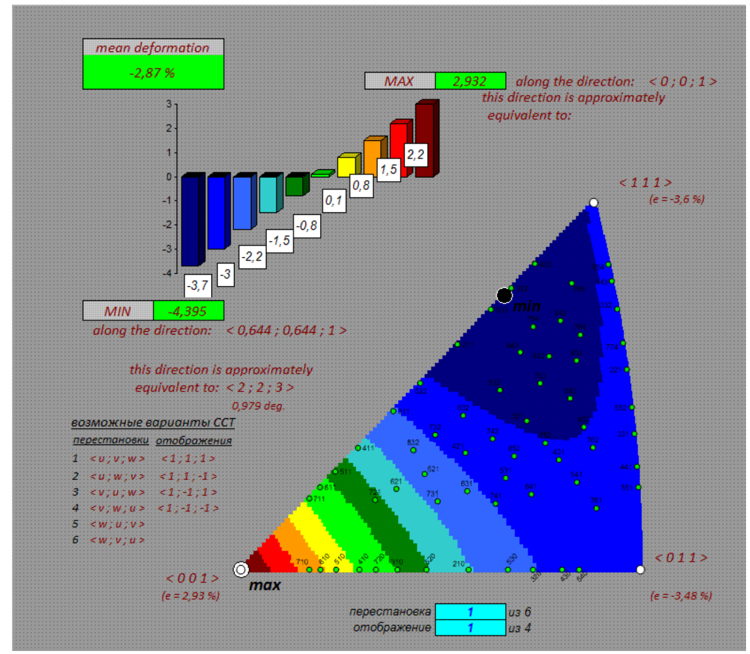
Engineering stress - engineering strain curve and evolution of phase composition during tensile deformation of ultra-fine grained.

- microstructure characterization (TEM, RSEM and XRD) of fabricated by severe plastic deformation (SPD-ECAP) nanostructured NiTi specimens and of specimens prepared via cold sintering

Results: mechanical and microstructural characterization of nano-NiTi, and synthesis of nanostructured NiTi foam

Task 2.3 and 2.4. Micro- and macromechanical (crystal lattice scale) modeling of martensitic deformation in Ti-Ni and Ti-Nb-based alloys with superelasticity and shape memory effect (MISIS)

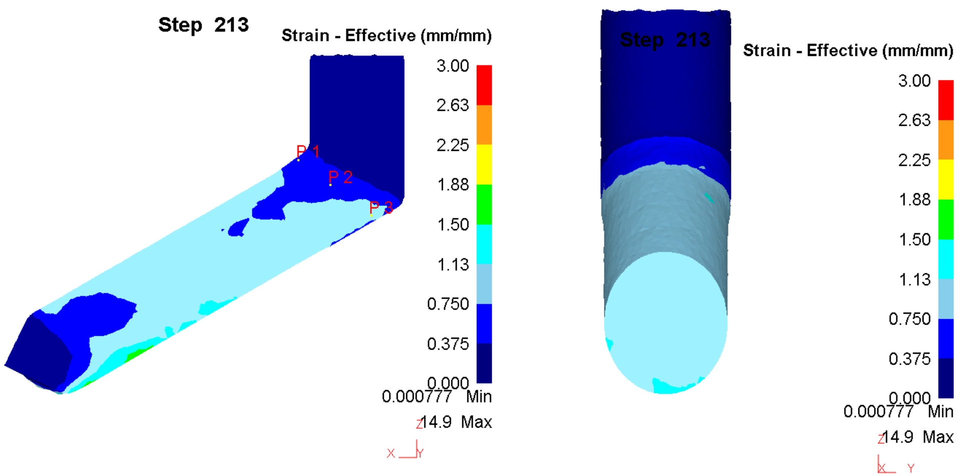




This program can construct a complete distribution of the stereographic projection of theoretical resource of shape recovery .

Results: methods and computer programs for determine a theoretical (crystallographic) resource of the recovery strain and crystallographic orientation of the maximum recovery strain based on the precise calculation of austenite and martensite lattice parameters

Task 2.6. FE modeling of the deformation, evolution of micro/dislocation structure for nTi-alloys with superelasticity and shape-memory effects under SPD(USATU)



Distribution of strain intensities during ECAP of TiNi in the longitudinal section of a billet

- ❑Modeling of material flow during SPD using Deform 3D software with account of technological parameters used in real-time processing for analysis of strain distribution in a billet and evaluation of formability for proposed processing modes.
- ❑Uniform distribution of strain intensities in a billet in the longitudinal and cross section

Results: development of a computational thermodynamics based model of martensitic phase transitions in nanonitinol, which includes effects of grain size, thermodynamical and mechanical properties

Task 2.7. Discrete-continual modelling of mechanical properties of metallic biomaterials, texturing, nucleation and plastic deformation under dynamic loading (ISPMS).

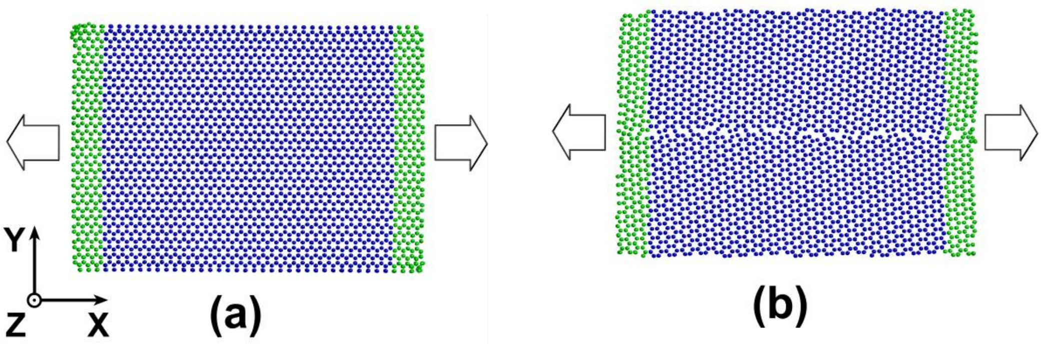


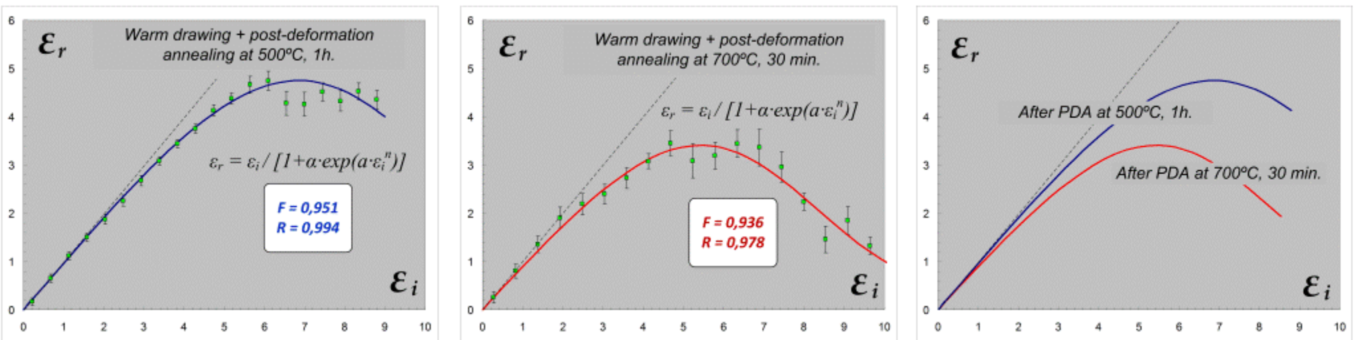
Fig. 2.17. Projection of the crystalline structure and the loading scheme of the simulated crystallites (a) crystallite having ideal structure;

(b) crystallite containing symmetric grain boundary which has misorientation angle α=53°

Potential energy of the tensile crystallite would increase monotonically with growing deformation.
When the threshold strain level is attained, the potential energy would no longer increase. Even though the extent of straining still continues to grow, the energy decreases in an avalanche-like manner. This effect is attributed to the initiation and development of plastic deformation.

Results: investigation of atomic mechanisms involved in the local structural transformations of the titanium crystallite in different mechanical loading conditions, using molecular dynamics method and parameterized semi-empirical Finis-Sinclair-type potential for Ti.

Task 2.8. Experimental validation of the modeling results. Samples of nanomaterials with shape-memory and superelasticity effect produced by different methods (MISIS).



(a) (b) (c)

Shape recovery parameters corresponding to treatments

Express-evaluation of shape recovery in SMA based on the precise analysis of real profile of sample in three states: initial (undeformed), after deformation (according to the scheme of the three point bending) and after shape recovery
a series of experiments on deformation parameters of shape recovery in samples made from Ti-50.0at%Ni carried out.

Results: experimental studies of microstructures evolution and shape recovery in SMA and the development of the method of express-evaluation of shape recovery in SMA

RELATIONSHIPS BETWEEN TASKS

T2.7 MD model of deformation of crystalls (ISPMS)

T2.1. Grain boundary sliding model of deformation of nanoNiTi (Technion)

T2.6. Modelling of materials flow and ECAP of nTiNi (USATU)

T2.3 Mechanical and structural haracterization of nanoNiTi (IMDEA)

Mechanical properties and production of nanoNiTi

T2.4. and 2.5. Crystall lattice model of SMA nanoNiTi and recovery strain analysis (MISIS)

T2.2. Micromechanics of martensitic transformation in nanoNiTi (DTU)

T2.8. Experimental study of structure evolution and recovery in nNiTi(MISIS)

SMA Effects in nanoNiTi

WP3. MODELLING OF BIOCOMPATIBILITY

WP3: Biocompatibility of nSMA & nTi

T3.1. Ion diffusion in body fluids (Techn)

T3.2. MD Model (FIAS, Techn)

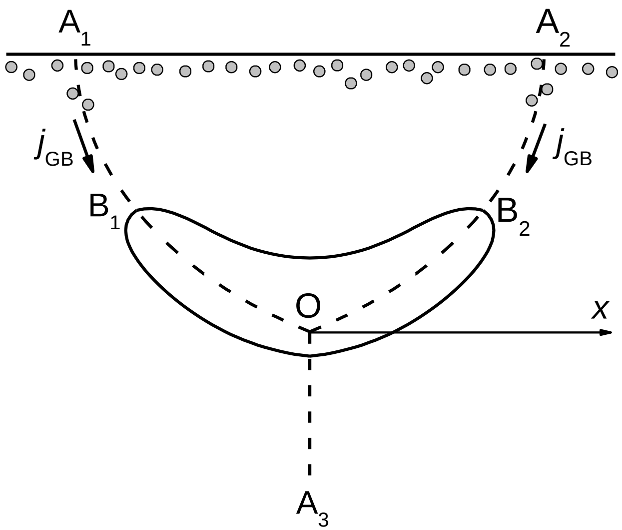
T3.3. GB diffusion (Techn)

T 3.4. Validation (Immersion) (Technion)

T3.5. Rheology (ISPMS)

T3.6. Electrochemical tests (MISIS)

Task 3.1. Theoretical modelling of dissolution rate based on ion diffusion from surface and grain boundaries of nanoTi and Ti-Ni (Technion)

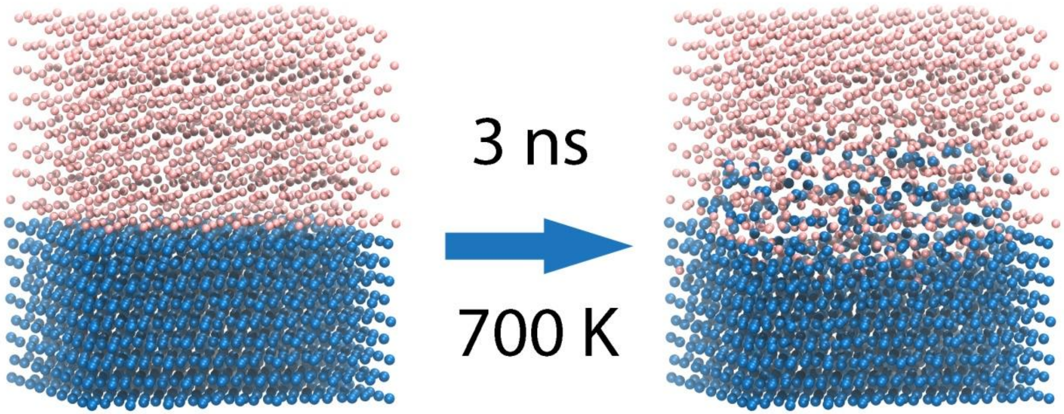


A two-dimensional subsurface pore growing due to the GB diffusion flux of vacancies, j_{GB}, from the surface where they are produced (by oxidation or anodic dissolution).

- ❑model for disintegration of nanostructured materials as a result of interfacial cavitation induced by vacancy supersaturation on the surface
- ❑excess vacancies produced on the surface of a polycrystal (by oxidation or anodic dissolution) may cause GB cavitation and pores growth in the subsurface regions of the sample
- ❑demonstrated that the pore growth is highly localized, with the narrow slits propagating along the GBs leading from the triple junction to the free surface.

Results: model of subsurface pore growth due the grain boundary diffusion flux of vacancies, which lead to the conclusion that excess vacancies produced on the surface of a polycrystal may cause GB cavitation and subsubface pore growth

Task 3.2. MD modelling of dissolution for ion diffusion from the surface and grain boundaries of nanostructured Ti and Ti-Ni SMA into body fluid (FIAS-GU)

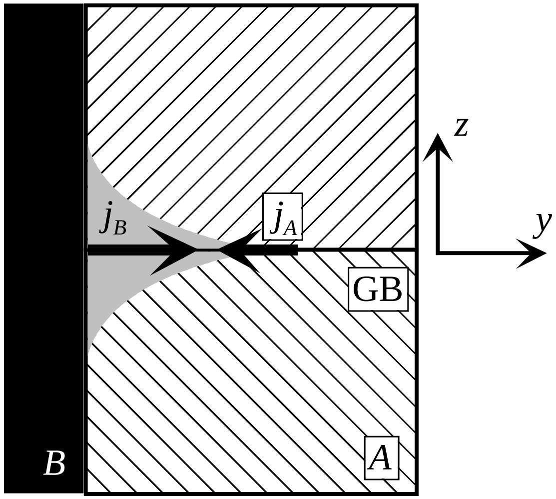


❑Evaluation of diffusion coefficients of Ni at different conditions

Initial and final structures of the Ni-Ti interface. Titanium and nickel atoms are shown by red and blue colors, respectively.

Results: development of molecular dynamics models of diffusion processes on interfaces of Nti and TiNi with fluids

Task 3.3. Theoretical modeling of Ti and Ni diffusion to the grain boundaries and along grain boundaries in nanostructured Ti and Ti-Ni shape memory alloy (Technion)

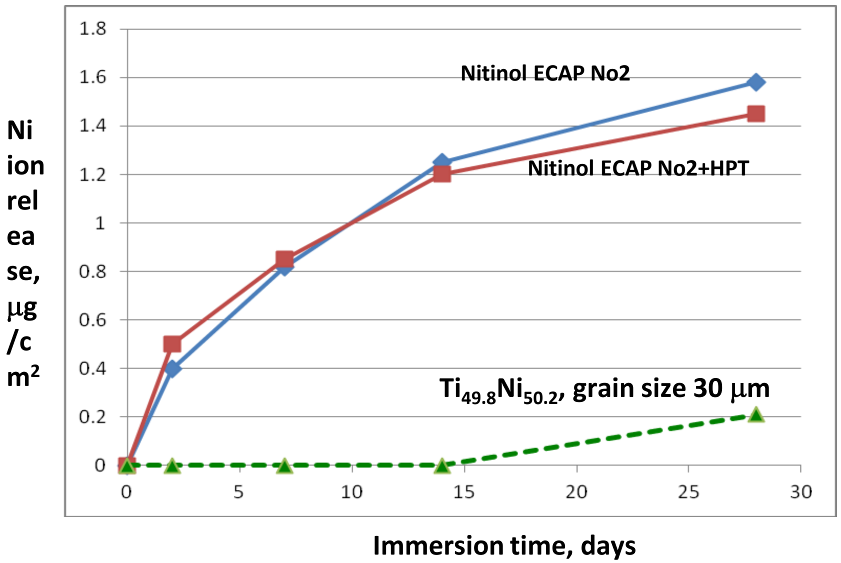


A bicrystal of *A* with the layer of *B* deposited on the surface. The imbalance of diffusion fluxes of the two components, j_A and j_B, is caused by the difference in intrinsic diffusivities of *A*- and *B*- atoms along the GB. This imbalance leads to the formation of an extra material wedge at the GB..

- Conclusion: the high-angle GBs are indeed efficient vacancy sources/sinks. The vacancies emitted locally by the GB in the course of GB interdiffusion process cause the formation of an extra material wedge at the GB.

Results: development of preliminary theoretical model of Ti and Ni diffusion along grain boundaries in nanostructured Ti and Ti-Ni shape memory alloy based on Kirkendall effect of grain boundary sliding, GBS

Task 3.4. Experimental validation of the biocompatibility modelling results. Measurement of dissolution rates of nanostructured Ti and TiNi in SBF - experimental validation (Technion)

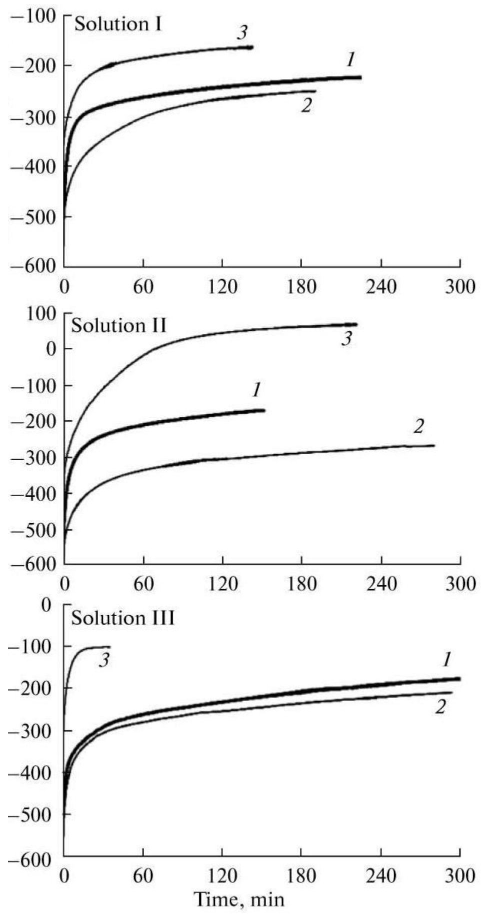


Ni ion release from conventional grain size TiNi alloy ($Ti_{49.8}Ni_{50.2}$, 30 µm) and nanocrystalline Nitinol ECAP No2 and Nitinol ECAP No2+HPT specimens as a function of immersion time

- Corrosion and electrochemical behavior of nanocrystalline and micron grain size pure Ti and NiTi samples was studied in Ringer’s solution which simulates physiological (body) fluid

Results: it was demonstrated that corrosion resistance and metal ion release of nanocrystalline Ti and NiTi alloy is at least as good as that of their conventional grain size counterparts

Task 3.6. Experimental validation of the biocompatibility modeling results (MISIS)

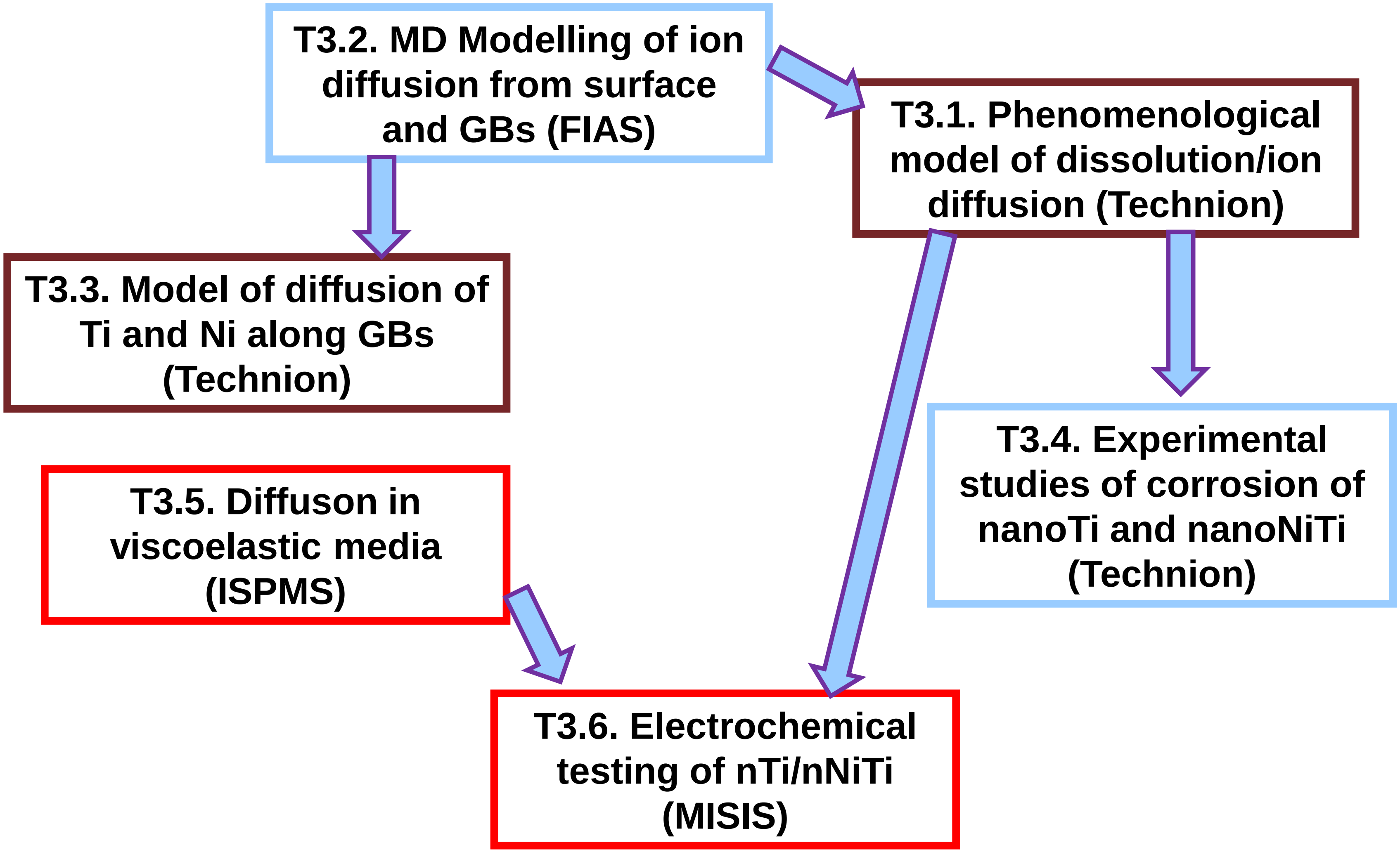


Typical OCP curves. Example in the figure – Ti-Nb-Ta in Hank's solution (solution I), saliva (solution II), acidic Hank's solution (solution III).

- ❑ The experimental samples were Ti-22Nb-6Ta and Ti-22Nb-6Zr (at. %) alloy; commercially pure titanium, Nitinol Ti-50.9Ni.
- ❑Simulated physiological solutions: 1) Hank's solution, 2) artificial saliva solution; 3) acidified Hank's solution, simulating traumatized condition of bone tissue, with HCl addition to adjust pH to 5.

Results: electrochemical tests of nanostructured Ti, TiNi and TiNb and experimental validation of modeling results using simulated physiological solutions

RELATIONSHIPS BETWEEN TASKS



WP4. MODELING OF NANOINDENTATION AND 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.

WP4: Nanoindendation and bioactive films

T4.1. MD model of nanoindentation (FIAS, Techn)

T4.2 PIRAC (Techn)

T4.3.Plastic deformation (nanoind.) (ISPMS)

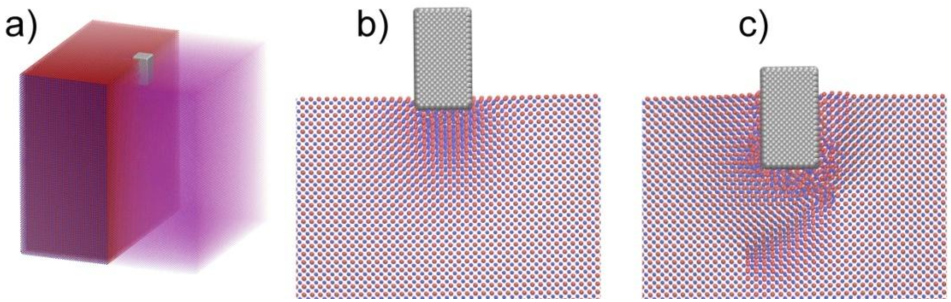
T4.4. Fracture of nTi/nSMA (nanoind) (MISIS)

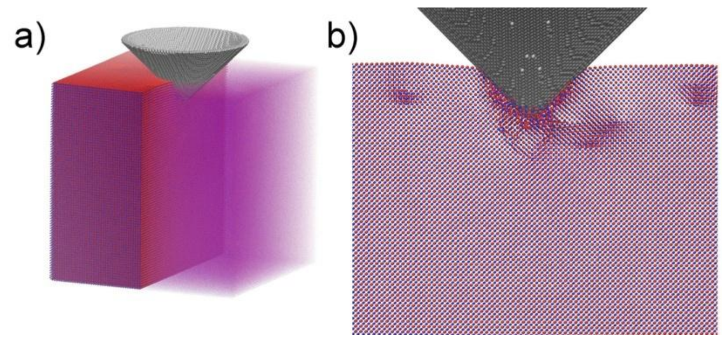
T4.5. MUBINAF wear (MISIS; IPMBS)

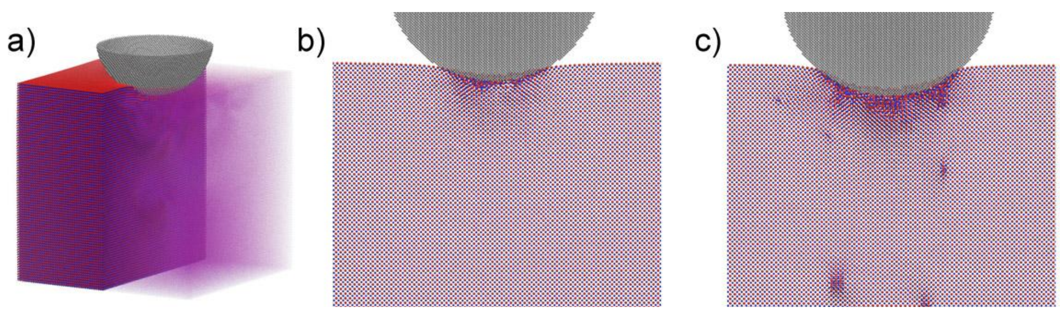
T4.6. Hierarchical model (ISPMS)

T4.7 Nanoindentation, scratch (MISIS)

Task 4.1. MD modeling of nanoindentation process of biomaterials and analysis of stress distribution and strength, including surfaces with grooves along grain boundaries (FIAS-GU)

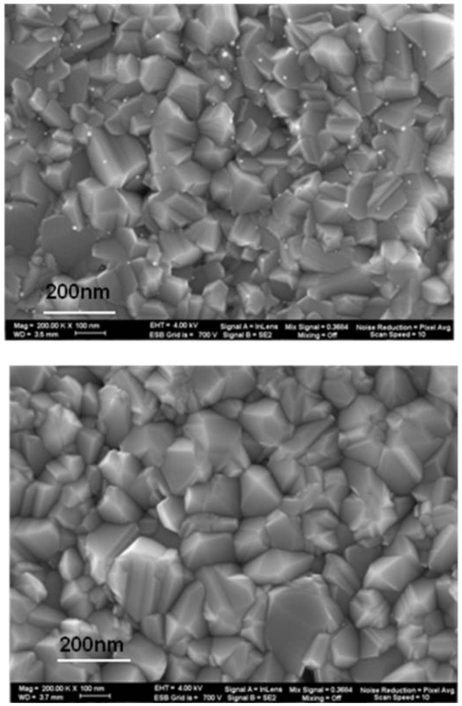






Results: large-scale (1 Mio atoms) MD simulations of the nanoindentation process of a bimetallic nickel-titanium crystal which allowed to identify the different deformation regimes depending on the geometry of the indenter

Task 4.2. Testing PIRAC Coatings (Technion)

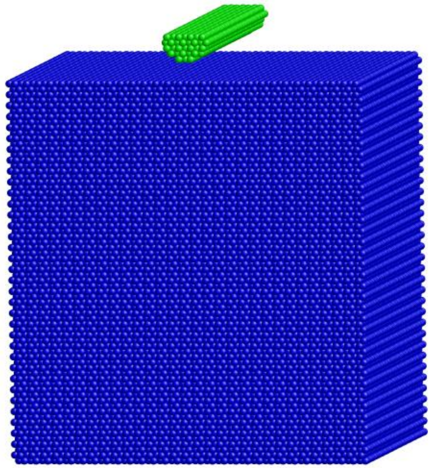


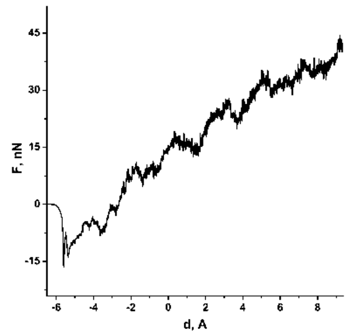
HRSEM of thermally etched at 600°C for 30 min cross section of nano-Ti: a) as received; b) after PIRAC nitriding treatment at for 100h at 600°C

- Results on PIRAC (Powder Immersion Reaction Assisted Coating) nitriding of nanostructured Ti based alloys at relatively low temperatures are presented.
- In PIRAC 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.

Results: it was demonstrated 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

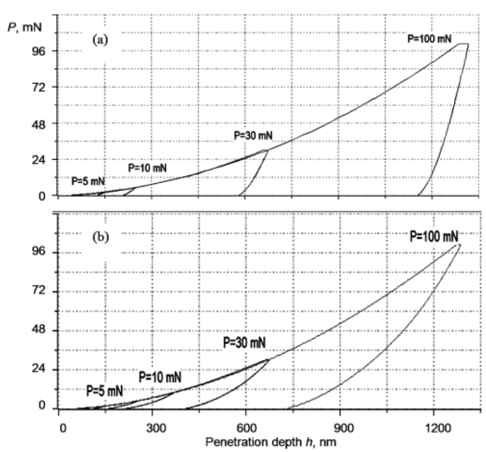
Task 4.3. Particle method based model of plastic deformation in metallic biomaterials under nanoindentation (ISPMS)





Result: development of particle based model of nanoindentation, and analysis of the deformation mechanisms and kinks in the nanomaterials.

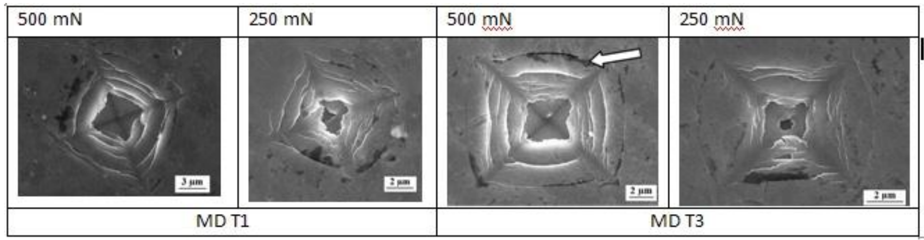
Task 4.4. Nanoindentation testing of three groups of Ti-based nanomaterials (Ti, SMA Ti alloy) (MISIS)



Indentation curves for the samples of (a) microstructured titanium **T1** and (b) nanostructured shape memory alloy **TN4** as taken at different loads P = 5, 10, 30, and 100 mN

Result: it was observed that for shape memory alloys (SMAs), the surface area between the load–unload curves is markedly lower while the elastic recovery, higher as compared to those for ms-Ti and ns-Ti

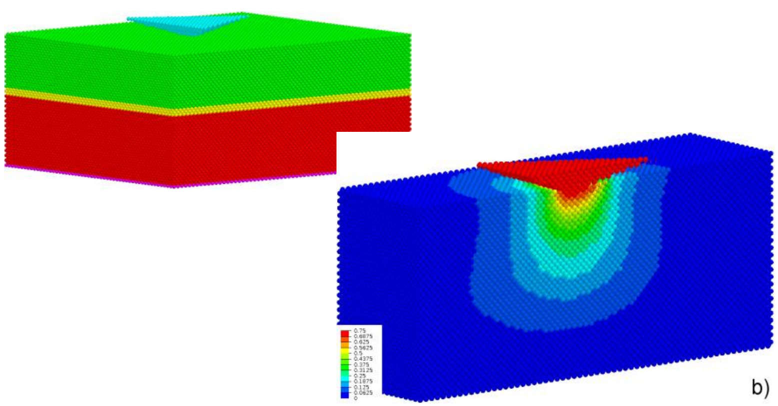
Task 4.5. Mechanisms of localized deformation of MUBINAF and protective wear resistant TiN coatings on the substrate of Ti-based nanomaterials (MISIS, ISPMS SB RAS).



SEM images of indents on the coated surface of ms-Ti (**MD T1**) and ns-Ti (**MD T3**) at the applied load 250 and 500 mN.

Result: the analysis of the effect of deposition of TiCaPCON multicomponent bioactive ns-films (MUBINAF) on the mechanisms of localized deformation and mechanical properties of nanomaterials.

Task 4.6. Multilevel hierarchical model of deformation and fracture mechanisms of nanocoatings on Ti-based materials (ISPM).



Result: MCA method based multilevel model of mechanical behaviour of heterogeneous nanostructured bioactive coatings on nanocrystalline Ti-based biomaterials developed

RELATIONSHIPS BETWEEN TASKS

T4.1. MD modelling of nanoindentation in nTi and nNiTi (FIAS)

T4.3. Particle method/analysis deformation mechanisms under nanoindentation in nTi (without coatings) (ISPMS)

T4.4. Nanoindentation testing of nTi, NiTi (without coatings) (MISIS)

Multiscale Model and Analysis of Nanoindentation in nTil/nNiTi

T4.5. Mechanisms of coating deformation and failure (MISIS)

T4.6. Multiscale model of deformation and strength of coatings (ISPMS)

T4.7. Experiments on indentation and dynamic loading of coated nTi/nNiTi(USATU)

T4.2. Graded coatings with good adgesion and wear resistance on nTi/nNiTi(Technion)

Biocoatings: Multiscale model and development

WP5. MANAGEMENT AND COORDINATION

COORDINATION/ MEETINGS

Working meeting of EU Consortium, 25.11.2011

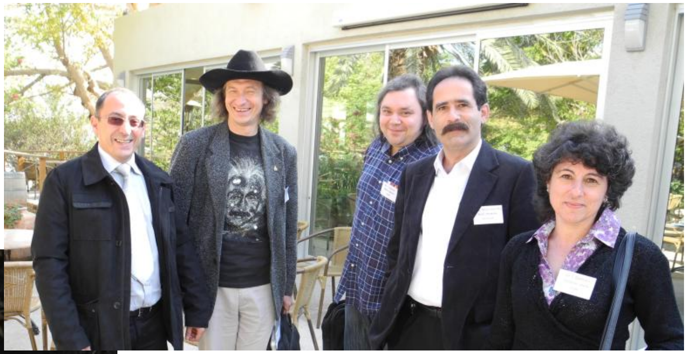
General Kick-off Meeting, 17.-18.01.2012

General Meeting, Moscow, 6-7 June 2012

3rd General Meeting and International workshop on

Nanostructured Ti based alloys for medical applications

Ein Gedi, 21-23.1.2012



4th Meeting and International Conference

SEVENTH FRAMEWORK PROGRAMME

Project funded by the European Commission under the 7th Framework Programme for Research and Technological Development in the framework of Theme 4 NMP - Nanosciences, Nanotechnologies, Materials and new Production Technologies – as a Coordinated call EU-Russia 2011

Project ViNaT
Contract No.: 295322

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

DTU

GOETHE UNIVERSITÄT FRANKFURT AM MAIN

International Conference on

COMPUTATIONAL MODELLING OF NANOSTRUCTURED MATERIALS

September 4-6, 2013
Frankfurt am Main, Germany

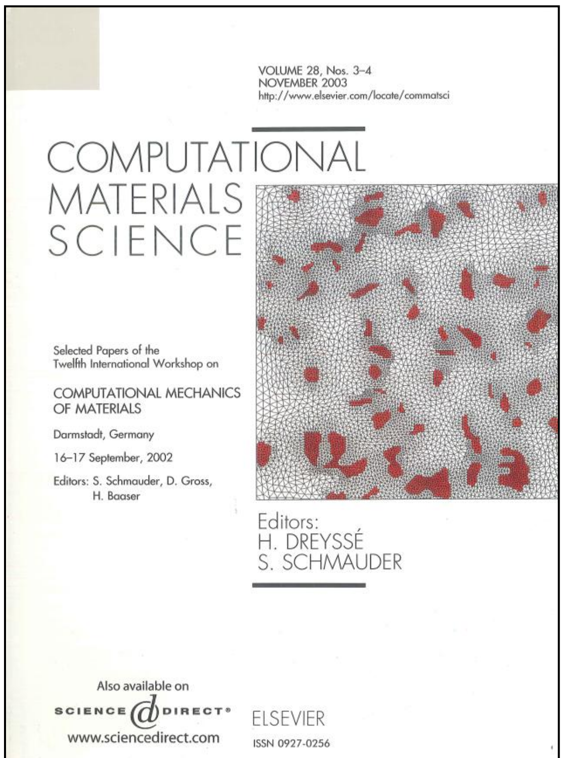
Contact:

Dr. habil. Leon Mishnaevsky Jr. (DTU, Denmark): lemi@dtu.dk
Prof. Andrey Solov'yov (FIAS, GU, Germany) mbn@fias.uni-frankfurt.de

SPECIAL ISSUE OF THE JOURNAL

COMPUTATIONAL MATERIALS SCIENCE

with publications from VINAT project



LIST OF PAPERS:

- L. Mishnaevsky Jr, E. Levashov, **Editorial**
- M. G.C. Seefeldt, A disclination-based approach for mesoscopic statistical modeling of grain subdivision in niobium,
- A. Verkhovtsev, et al, Computer simulation of diffusion process at interfaces of nickel and titanium crystals,
- A. Verkhovtsev et al., Molecular dynamics simulations of nanoindentation process of titanium crystal,
- L. Klinger, I. Gotman, E. Rabkin, A mesoscopic model of dissolution/disintegration of nanocrystalline metals via vacancy diffusion along grain boundaries,
- I. Sabirov et al, About application of three dimensional analyses of fracture surfaces in fracture study on nanostructured titanium,
- R. Chembarisova, I. Alexandrov, Analysis of deformation behavior mechanisms in ultrafine-grained Ti grade 4,
- H.S Liu, L.Mishnaevsky Jr, Martensitic transformations in nanostructured nitinol: FE modelling of grain size and distribution effects,
- J. Segurado, Simulation of the deformation of polycrystalline nanostructured Ti by computational homogenization,
- W. Pantleon, Work-hardenings stages and deformation mechanism maps during tensile deformation of commercially pure titanium
- A. Smolin et al, Modeling nanoindentation of TiCCaPON coating on Ti substrate using movable cellular automaton method,

WP6. Recommendations and technical specifications of new materials, their testing and control

WP6: Technical specifications

T6.1. Patent analysis (MISIS)

T6.2. Recommendations for the production nTi/nSMA based materials with coatings (USATU, Nanimet, ISPMS)

T6.3. Control quality of new materials Nanomet, Metal)

T6.4. Market potential (MISIS)

T6.5. Technical specifications (Nanomet, Metal, USATU, MISIS, ISPMS)

SOFTWARE DEVELOPMENT

LINK:

http://gr01.misis.ru/vinat/

SOFTWARE includes modules

Multi-scale modeling of nTi

1.Module for a wide-scale molecular dynamics (MD) simulation of strain processes and structural transformations in nTi. (FIAS)

2.Module for calculation of parameters for microstructure and stress-strain properties of nanostructured TiNi alloys (IMDEA)

3.Module for the express evaluation of mechanical properties of nTi (DTU).

Multi-scale modeling of nSMA

1.Express evaluation of fraction of martensite under loading (DTU).

2.Crystal lattice modelling of SMA (MISiS)

3.Martensitic deformation (MISiS).

4.Microstructure evolution: (USATU)

5.Module for multiple-level modeling of plastic deformation initiation and growth in metallic materials under complex stress-strain load (Monster-PT). (ISPMS)

Biocompatibility of nSMA & nTi

1.Module for GB diffusion modeling (Technion)

2.Module for modeling of multi-component diffusion in solid solutions. (ISPMS)

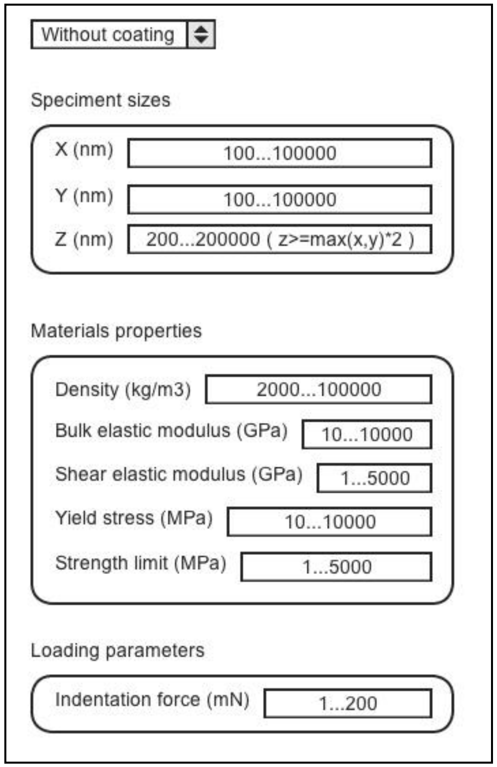
3.Module for large-scale MD simulation of diffusion processes. (FIAS)

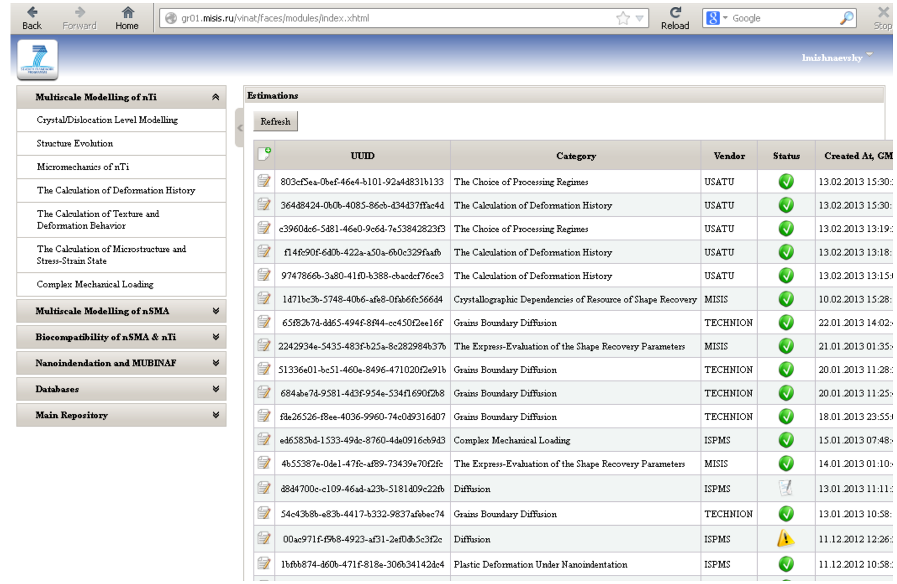
Nanoindendation and bioactive films

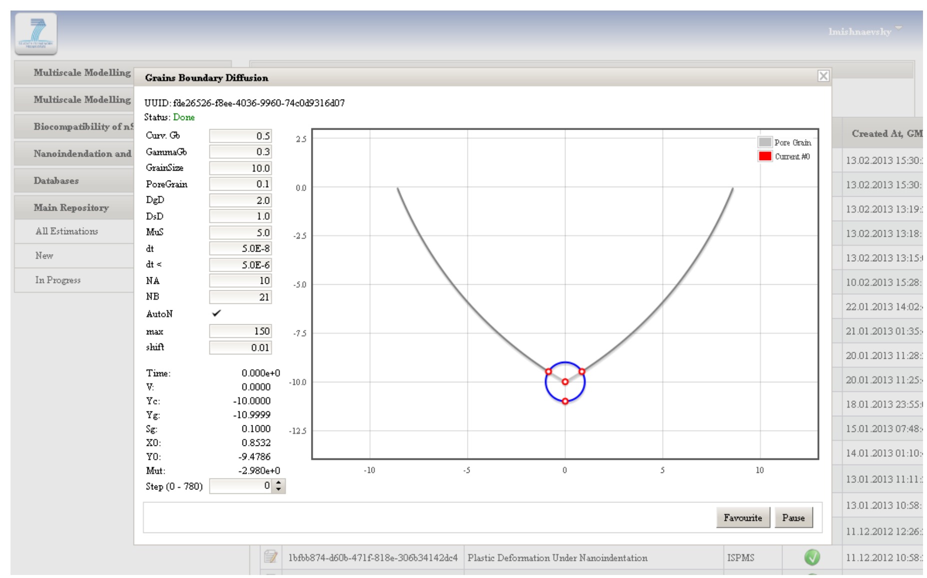
1.Module for multiple-level modeling of metallic materials indentation. (ISPMS)

2.Fracture of nTi/nSMA (nanoind)(MISiS)

SOFTWARE: Screenshots







Form for entering input parameters of multiple-level modeling of birth and development of plastic deformation in metallic materials under complex stress-strain load (Monster-PT) (instead of Indentation force – Loading force)

Schreenshots of software complex

MAIN RESULTS

- **Multiscale model of mechanical behavior and biocompatibility of nano-Ti**, including atomistic dynamic modelling, polycrystal homogenization, micromechanical dislocation density based model, dislocation based texture and defect evolution, grain boundary sliding effect, and validation;

- **Multiscale model of mechanical properties of UFG shape memory Ti-Ni alloys**, taking into account the grain size effect on martensitic transformations, crystal lattice phase parameters, share recovery parameters, and validation;

MAIN RESULTS

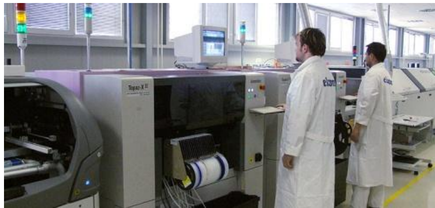
- **Modelling of biocompatibility of nTi and Ti alloys**, including MD + phenomenological analysis of ion diffusion from surface and grain boundaries, and validation
- **Multiscale model of nanoindentation testing**, including MD simulations of nanoindentation with different indenters, particle methods modelling, coating analysis and development, and validation;
- **Patent analysis,** development laboratory instructions for testing, economical evaluations of market potential of the developed software and materials;
- Concept and some modules of the s**oftware for multiscale virtual testing** of nanostructured Ti and Ti-alloys

Expected Final Results:

- **Complex of advanced computational models**, allowing the analyze the mechanical behavior and biocompatibility of nanostructured metallic materials at the atomistic, dislocation and microstructural scales,

- **Modular software complex for virtual testing of nanostructured** for medical applications,

- A number of **production technologies** for nanostructured materials with required, improved structures, and **advanced testing procedures** for the model validations.



Potential Impact:

- ➢efficient, reliable and **quick development of biocompatible nanometallic materials**, with minimum tests, also animal tests

- ➢Exploring and finding **new reserves of improvement of production technologies** and materials properties

- ➢**new possibilities in trauma surgery**, orthopaedic and oral medicine, with possibilities of healing bone illnesses, dental problems, traumas at the new level ->
Many people, who suffer from the bone or dental diseases now, can be brought back to active life.

- ➢Leading to the creation of a **new quickly developing industry branch**.

THANK YOU FOR YOUR ATTENTION!

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