MODELING OF THE NANOSTRUCTURING MECHANISMS IN SEVERE PLASTIC DEFORMATION OF THE CRYSTALLINE MATERIALS BASED ON THE LIVE CELL MIMICS

Objectives

At the nanoscale size (under 20 nm), the dislocations interact in a complex way, revealing three mechanisms: (1) dislocation cutting processes, jog formation and generation of trails of point defects, (2) activation of secondary slip systems by Frank-Read and cross-slip mechanism, and (3) formation of sessile dislocations such as Lomer-Cottrel locks.

It was discovered [1,2,5] a new class of point defects as trails of partial point defects which could play an important role in situations when partial dislocations dominate plasticity. The geometric arrangement (fig. 2) explains the particular structure that is almost similar with the folded protein chains. By comparison, in fig. 2 it could be noticed the similarity of the folding state of the protein (b) and the dislocations (a) that appear as the wiggly bluish lines in the plot. Moreover [4], the study of the response of a tropocollagen molecule under tensile force (c) has shown that its deformation is controlled by entropy in the first stage, at a critical value of the applied force the molecule becomes straight, when energetic elasticity starts to dominate. This deformation continues until the molecule ruptures. After the molecule has rupted, the free molecule starts to entangle again, due to the lack of applied force. It is considered also a persistence length at which the molecule stands straight. Such of a deformation mechanism sounds like the deformation mechanism at the microscale in crystalline materials where the Frank-Read sources acts as a driver of plasticity.

This analogy is the key idea in identification the deformation mechanism in the Region IV of fig. 1 where is a lack of explanations how nanometals deform.
To substantiate this approach it is necessary to analyse in more detail the deformation mechanisms and driving forces acting in proteins, such as chemical interactions, reactive force fields, elastic entropy, and to partly use this analogy in developing a simplified model for the deformation of ultra-fine nanocrystalline materials. A combination of these weighted effects with the cooperative grain boundary sliding could explain the deformation mechanism of the nanometals.

One essential point that should be verified is that the state of the nanometals is quasi-amorphous, because the biological materials and rubber, the reference for the proposed material modeling, are characterized by a great degree of disorder (amorphous state), which is measured by the entropy. When such materials are deformed, the entropy decreases, while when removing the external forces, the entropy tends to increase to its initial level. This is the so-called elastic entropy. In a meso-crystalline structure, the dislocations move along preferential planes and directions, while in nanocrystalline materials the main deformation mechanism is the grain boundary sliding accommodated by partial dislocations that look like and possibly behave in the same way as molecular chains.

The goal of the project: the project goal is to control the deformation mechanisms in nanometals that will open new opportunities: 1) to design new technologies for metal forming that gives ab initio improved mechanical properties as superplasticity, wear resistance and magnetism, 2) conception of the new constitutive modela of the materials necessary to dynamic modellling of the SPD processes with high precision 3) application of the self-organising principles in designing of the small devices for medicine, mecatronichs and nanomechanics.

The major objective of the project: The method to achieve the proposed goal is to develop a new model of the deformation mechanism encountered in severe plastic deformation that is based on the analogy from celullar biology where the movement of the protein chains can have common points with the movement of the trails of the point defects dislocations. With this analogy we can control the relation between mechanical properties of the macroscale material and its bevaviour at the atom-scale.

The specific objectives of the project:

Objective 1 - Identification of physics phenomenology dislocations behavior at the activation of the second slip system that corresponds nanostructure at grain size of 20nm

1.1.Synthesis of deformation mechanisms presented in specialty literature with very high impact factor and determination of pressure conditions and deformation degree at which takes place the nanostructuring.

1.2. Identification of displacement patterns of the tubes for vacancies for the materials: Ni, Cu, Al-Mg, Ti through the modeling technique ARMA model (autoregressive moving average models)

1.3. Identification of the relationship between grain size at which the second slip system is activated and the pattern for tube vacancies. (dislocations)

Objective 2 - Study of deformation mechanisms of the actins chain from the proteins

2.1.Statics identification of protein chains possible candidates in the analogy with crystalline nanostructured network obtained by severe plastic deformation processes.

2.2. Investigation of internal dynamics in the proteins constrained to mechanical action by one side, and evolution

of dislocations in nanocrystalline – nanometals materials, by the other side.

2.3 Synthesis of deformation mechanisms (folding/defolding) in aminoacids chains from the selected proteins.

2.4 Analysis of investigated probes similarity and extraction of the results necessary for modeling.

Objective 3- Mathematical modeling of the deformation mechanisms identified at the selected proteins

1.1. Mathematical modeling in mechanical and biochemical conditions that characterize kinematics of proteins chains.

1.2. Determination of periodical conditions which restrict grain frontiers.

1.3. Equation synthesis that describe kinematics of proteins chains.

1.4. Evaluation of nature weight in deformation mechanisms

Objective 4 - Modeling the evolution of nanostructuring in similar conditions of a deformation with ECAP process (Equal Channel Angular Pressing) of the ultra fine grain materials using cellular copy with circular section of Ø5 mm. 3.1. Creating the model in molecular dynamics based on the equations that describe chain kinematics-creating the model.

3.2. Establishing conditions at grain frontiers.

3.3.Modeling with the help of molecular dynamics for 5 grains having a progressive number of 30000-100000 atoms.

Objective 5 - Characterizing the internal state of the nanostructure by identifying state variables.

1.1. Identification of the relationship between the elastic entropy, density of dislocation and the nanostructure mechanism- conceiving the appropriate state variables.

1.2.Identification of relationship between energetic potential of atoms from the interface of two grains and the position of partial disturbance lacks.

Objective 6 - Coupling the model at nano scale with the nanostructuring macro model by ECAP competitive multiscalar analysis.

2.1. Identification of state variables that characterize evolution of grain frontiers geometry in similar conditions with nanostructure ECAP process (Equal Channel Angular Pressing)

2.2. Conceiving identification algorithm of coefficients values that describe the state of variables by numerical or experimental tests.

2.3. Determination of coefficients value for internal state of variables for Cu, Ni in ECAP case.

Objective 7 - Macroscopic modelling of material's behaviour during severe plastic deformation ECAP.

3.1. Developing internal state of variables in structural analysis program with finite element V-STRUCT

3.2. Identification of coefficients values that characterize the state of variables by molecular dynamics.

3.3. Numerical modeling of a piece obtained by ECAP.

Objective 8 - Simulation and validation of hypotheses and multi scalar characterization of nanostructured materials Cu, Ni.

1.1. The experimental accomplish of a plastic deformation die by ECAP process.

1.2. Microscopic analysis TEM/SEM/HSTEM/AFM of the obtained microstructure by peak broadening and measuring the elastic energy.

1.3. Comparing the numerical and experimental results.

Importance of the project for metal forming domain: The research in plastic behavior of materials has experienced clarification of the mechanisms of plastic deformation and the work-hardening of crystalline materials, carried out by solidstate physicists and the engineering structural analysis based on the phenomenological relationships - the so-called constitutive equations which represents the average over space and time scales that are many orders magnitude than the underlying elementary events of platic deformation. Recently, by developing the new technologies (SPD) and by developing computer power, new challanges occur in explanation of how materials behave at the atomic scale and what is the influence on the macroscale behavior? The project proposes to answer to this question and to ellucidate the origin of the deformation mechanism in the nanostructured materials obtained by ECAP process of severe plastic deformation that 1) allow the control of the processes to transform cristalline materials from low mechanical to high quality mechanical properties, 2) to design new processes that use the capability of the material to be deformed at high strains and 3) to allow new developments in the coupling the nano and macro scale analysis to a better prediction of the manufacturing of the parts within finite element simulation.
The importance of the project is underlined by the researches carried out in the famous laboratories in the field and the results are published mainly in Science and Nature reviews that have the greatest impact factor as ISI journals

Interdisciplinarity of the project
The *project is a transdisciplinary development* that include approaching of a unitary and complex phenomenon using the knowledge from physics, chemistry and mechanics combined, *in a novel and nonconventional way with genetics and cellular biology*. The research consist in using knowledge from continuum mechanics, cell biology and histopathology, industrial engineering, mechanics, informatics to put together to find a model of deformation mechanism at the nanoscale that will be largely used by future research in developying nanociences.