Thematic Proposal for **'Current Nanoscience'**

"Application of Molecular Dynamics simulations in nano-manufacturing"

Guest Editor: Dr. Angelos Markopoulos

Aims & Scope: During the past decade, developments in the area of nanotechnology have been extremely high and the applications have been continuously growing in numbers. Miniaturized mechanical parts, that can be used in a wide range of applications, including medical equipment, aerospace, computer systems, can now be produced using state-of-the-art, high-technology equipment. The thorough study and investigation of ultra-precision, nano-metric manufacturing processes involved in the production of parts, as well as all the phenomena that appear at this scale, have become a necessity. Experimental studies can be extremely costly and may not be sufficiently efficient for the aimed sub-micrometer dimensions. Nano-scale manufacturing involves interaction with the workpiece in a few atomic layers below the workpiece surface. On this scale, continuum mechanics computational methods, like the finite elements method, are not preferred. Instead and in order to gain a deeper understanding of microscopic material behavior and structure, Molecular Dynamics (MD) simulations are widely accepted. MD simulations use atomistic models that can be applied to study various material phenomena. The more universal material representation that MD simulations offer, considering lattice constants, orientation, microstructure, chemical elements and the atomic interactions, allows the researchers to go beyond ideal structures and homogeneous material properties and to describe poly-crystals, defect structures, pre-machined or otherwise constraint workpiece models and non-smooth surfaces with extreme accuracy.

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