Scientific Report for ESF Short Visit Grant NATRIBO-550
by Prof. Vladimir Pokropivny
to the Helsinki University of Technology (HUT), from 17 June to 01 July, 2005

Purpose of the visit was to extend multi-scale models of nanofriction, nanoseizure, nanobilliard and other nanotribology contact phenomena on case of complex MeX compounds .

During visit the following **work** was carried out and the **main results** were obtained:
1. Combined MD/TM model for multi-scale computer nodeling of nanofriction in nanotribology contact phenomena was further developed and extended on case of complex MeX (Me = metal, X = C, N, B, O) compounds. In this model the interatomic interactions of friction pair play a key role combining electron density empirical calculation, molecular dynamics (MD) simulation and calculation of friction coefficient at atomic level with theoretical mechanics (TM) modeling of tip-surface contact phenomena at microscopic and mezoscopic level. Output parameters of the theoretical model was connected with results of experimental TEM/AFM observations.
2. Model of mixed interatomic potential for MeX ceramic compounds was developed. As typical example a mutual consistent set of empirical interatomic potentials for TiB_2 diboride was designed including Ti-Ti, B-B, and mixed Ti-B potential of Buc-kingam and Mee-Gruneisen type. Discompensation of interatomic forces at unperfect deformation region was found in first time to result in latent internal stress leading to inherent brittleness of ceramics. This mechanism must be accounted in nanotribology to prevent tip fracture.
3. Computer code for simulation of contact phenomena in AFM was updated with account of this mixed potentials.

In result of the visit the joint **publication** preliminary named “Mixed interatomic potentials for multi-scale modeling of nanofriction in ceramics”
by V.V. Pokropivny, A.Lohmus, R.Nieminen have been prepared.

Together with Dr. Ants Lohmus from Institute of Physics ,University of Tartu**,** who has visited Helsinki University of Technology ,we have discussed and planned further **collaborative** research .
In the result of such previous collaboration within the NATRIBO-352 Exchange Grant in 2004 the INTAS **project** was submitted in 2005.

The result of the reserach were **presented** at NSF Conference "Molecular Crystal Engineering" held in Helsinki.

Dr. Vladimir Pokropivny