Scientific Report for ESF Exchange Grant Natribo-352
by Prof. Vladimir Pokropivny
to the Institute of Physics, University of Tartu (IPUT),
from Aug. 2 to 30, 2004

Purpose of the visit was to develop multi-scale models of nanoseizure, and other nanocontact phenomena**.**

During the visit the following work was carried out:
1. Interatomic potentials for model Cu metal and model TiC carbide was developed, the parameters of which were fitted to the set of crystal characteristics.
2. Computer programs for computer simulation of friction processes were modified and updated for account for the model metal and carbide.
3. Models of the nanoscizure and nanomanipulation at atomistic and mezoscopic levels were interconnected in the manner when the parameters of friction coefficients obtained in molecular dynamics atomistic simulation have to be used as the parameter in the finite-element method at the mezoscopic level.

The main result of the visit is the background was founded for further joint research of nanocontact phenomena combining multi-scale modeling with AFM/TEM experimental research.

Future collaboration with IPUT and Tallinn University is planned to be developed within the joint projects, entitled NANOSEIZURE and HYPERSOUND, the first version of which was prepared.

Together with Dr. Ants Lohmus we have made a short visit to Prof. Risto Nieminen in Helsinki University of Technology. In the result the joint publication preliminary named “Development of multi-scale models of nanoseizure, and other contact phenomena” by V.V. Pokropivny[1], A.Lohmus[2], R.Nieminen[3] is in the focus.

In IPUT the seminar entitled “New trends in advanced nanomaterials. Short review, original ideas, and promising applications” have been presented.

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Dr., Prof.