

An Appreciation of Allan Grivtsov (1937-1991)

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Allan Grivtsov died on the 12th January 1991. Born on April the 15th 1937 in Moscow, he was one of the pioneers and enthusiasts of molecular dynamics simulation. Allan was a student of the Chair of Biophysics headed by Professor L A Blumenfeld when the idea of molecular dynamics simulation came to him. At that time he did not know that this method had already been used by other scientists. He approached S E Shnol, lecturer in biochemistry, a very broad-minded scientist and a man of deep understanding of the problems of natural sciences (it was he who proposed to his student A M Zhabotinsky to study Belousov's reaction) for advice. S E Shnol said his brother, E E Shnol, a mathematician, got interested in the problem. The first of A Grivtsov's works on molecular dynamics simulation is an unpublished report (37 type-written pages), written by him in collaboration with E E Shnol in 1967. Its title was "On the numerical modelling of the molecular motion in a liquid". A Grivtsov started to propagandize the method. He spoke at various scientific conferences (some of his remarks were published in the discussion sections of the conferences' proceedings) trying to stimulate the interest of the specialists in various fields. After the discussion at the conference on the theory of adsorption he became a scientific worker of the Institute of Physical Chemistry. He performed, as far as I know, the first works on simulation of structuralisation of liquid near the solid wall and of adsorption. He was one of the first who used molecular dynamics simulation to study motions in a polymer chain. His candidate (Ph.D. equivalent) thesis, written in 1973 was entitled "Numerical experiments on modelling motions of the molecules". Soon, just after publication of Rahman and Stillinger's work he elaborated an original, very efficient algorithm for simulation of rigid multiatomic molecules and wrote a programme to simulate water.

A Grivtsov simulated dislocations in crystals, the deformation of a molecular crystal,

dynamics of the polymer crystal, studied influence of impurity on the strength of a crystal and performed many other excellent pioneering works. He delivered lectures, organised seminars, workshops and schools. Due to this activity computer simulation became rather popular in the USSR. I would like to mention four workshops on the application of mathematical methods to study of polymers. At these workshops, which took place in Pushchino (a scientific centre to the South from Moscow), the efforts of mathematicians, theoreticians, molecular biologists and polymer scientists were united. For several years he headed a very prestigious seminar on the computer simulation of polymers and condensed matter at Moscow University. It is impossible to enumerate all the scientific events in organisation of which A Grivtsov took part.

A Grivtsov had many disciples. He taught them to be strict in formulation of the tasks and the methods chosen to fulfil them. He thought a lot about fundamental principles of computer simulation and his contribution to their development was invaluable.

His favourite creation was his group in the Institute of Physical Chemistry. By and by after hard efforts and struggle it turned into the Laboratory of Mathematical Modelling of the physico-chemical processes. He passed away when he was 53 years old.

A list of A Grivtsov's publications comprises more than 70 items. For the most part they are abstracts, short communications and preprints, almost all in Russian. This brilliant scientist knew foreign languages rather poorly. Best of all he could read and speak in Esperanto, but few scientists are fluent in this artificial language and there is practically no scientific literature in it. It is one of the reasons why he is not as well known in the world as he deserves to be. The main reason was his modesty and the difficulty of travelling abroad for a real scientist during the years when he was in his prime.

List of main publications of Allan Grivtsov

1. On the structuralization of liquid near the solid surface. *Doklady Akademii Nauk SSSR* v.190, N4, p.868, 1970
2. Numerical modelling of the deformation of the molecular crystal. *Ibid.*, v.215, N1, p.148-151, 1974 (with V S Yushchenko and E D Shchukin)
3. Numerical modelling of the motion of a linear polymer chain. *Ibid.*, v.220, N5, p.1096-1098, 1975 (with N K Balabayev and E E Shnol)
4. On the analysis of the mechanism of the adsorbational decrease of the strength. "Fiziko-khimicheskaya mekhanika materialov" N1, p.31, 1976 (with V S Yushchenko)
5. Stability and dynamics of a drop on the solid state surface. "Kolloidnyi Zhurnal", v.39, N2, p.335-338, 1977 (with V S Yushchenko and E D Shchukin)

6. Heterogeneous crystallization (Kinetics and computer simulation). A book. (with D Fedoseev and P Chuzhko) Moscow, Nauka, 1978 (A Grivtsov wrote a chapter about molecular dynamics simulation - one of the best manuals in the world)
7. Geometrical sense of the temperature of the ergodic system. Zhurn. Fizicheskoi Khimii, v.54, N1, p.250, 1980
8. Molecular dynamics study of the distribution of the kinetic energy in the polyethylene molecule. Vysokomolekulyarnye soyedineniya, v.23b, p.121-123, 1981 (with N K Balabayev)
9. Numerical modelling of rotational crystalline states of the n-parafin Doklady Akademii Nauk, v.227, N2, p.412-415, 1984 (with M A Mazo, N K Balabayev et al)
10. Diffusion of the molecules in narrow pores. Kolloidnyi Zhurnal, v.5, p969, 1982 (with L A Grivtsova, N V Churaev, L F Chuikova)
11. Numerical modelling of protein molecular dynamics. Molekulyarnaya Biologiya, v.17,N3,p.587-616,1983 (with G G Malenkov and L V Abaturv)
12. Mathematical modelling of the adsorbtiional processes In: Adsorbtsiya i adsorbenty, Moscow, Nauka, 1987, p.81-87
13. Geometrical criterion of the hydrogen bond in computer simulated water. Zh.Strukturnoi Khimii, v.28, N2, p.81-85, 1987 (with G G Malenkov and M M Frank-Kamenetskii)
14. Molecular dynamics simulation of the vitrification of two-dimensional Lennard-Jones fluid. Rasplavy, v.1, N6, p.101-106, 1989 (with M I Kotelyansky and M A Mazo)

All these publications are in Russian. English translations of the most part of journals are available.

Below I give the full list of A Grivtsov's publications in English, including abstracts:

1. Mechanical behaviour of solid polymer - imitation by molecular dynamics method In: Molecular Mobility in Polymer Systems. P.336. Leipzig, 1981 (with N K Balabayev et al)
2. Molecular dynamics simulation of motion in solid polymers rotation phase of n-alkane. Polymer Bull. v.12, N4, p.303-309, 1984 (with M A Mazo, E F Oleynic et al)
3. Molecular dynamics simulation of the n-alkanes rotator phase In: Physical optics of dynamic phenomena and processes in macromolecular systems. p.413-425, Berlin, 1985 (with M A Mazo, E F Oleynic et al)

4. Molecular dynamics simulation of water: adsorption of water on -tridimite. J. Coll. Interface Sci., v.126, N2, p.397-407, 1988 (with L T Zhuravlev, G A Gerasimova and L G Khazin)
5. Molecular dynamics simulation of liquids contacting the solid surfaces. Symposium on the structure of liquids and solutions August 24-27. Vespem. Abstracts p.37-39, 1987
6. On the thermodynamically correct molecular dynamics simulation of water. International conference on solution chemistry. Jerusalem August p.102, 1989 (with M M Frank-Kamenetskii and D L Tytik)