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In-person: NOMATEN seminar room, NCBJ

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Molecular Dynamics simulations of stress propagation and dislocations in crystals: example of Fe-Ni-Cr steel.

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Abstract:

Simulations in molecular dynamics (MD) often are carried out in an applied pressure, as for instance in case of modelling the dynamics of dislocations in materials. In analysis of results a crucial role is played by the proper understanding of underlying process of pressure penetration itself, since this is a dynamic process occurring at the same time scales as the studied properties of material.

Movement of line dislocations in FCC steel 310S is found to depend on the size of nanometer sized structures. The effect is attributed to time (and size) dependencies of pressure propagation into the medium. The observation is crucial in interpreting any MD studies of pressure effects since these are governed by time-dependent internal virial stresses. In particular, velocity of dislocations scales better with value of local internal shear component of virial stress than with external shear pressure applied.

In this presentation I will focus on technical aspects of stress field propagation into material interior, illustrating the results by analysis of the dynamics of line dislocations..

Bio:

Zbigniew Koziol graduated with M.Sc. from Physics Department of Warsaw University, with a thesis "An Investigation of the Magnetic Properties of CdMnTe by Optical Methods". In years 1986-1990 performed experimental research in Institute of Physics, Polish Academy of Sciences, in a laboratory of "Magnetism and Magnetic Materials". In 1994 awarded a Ph.D. degree from Van der Waals-Zeeman Laboratory of Universiteit van Amsterdam, after 4 years of experimental research documented in thesis "Superconductivity in Heavy Fermion and Copper-Oxide Systems". As a Killam Memorial Postdoctoral Fellowship at Physics Department of Dalhousie University in Halifax, Canada in 1995 he continued work on superconductivity and participate in investigations of giant magnetoresistance in quasi-crystals. For over 12 years engaged in Canada in activities related to the Internet development, programming, open source and Linux, forming his background for technical excellence in using computers for scientific research. In years 2008-2013 worked on computer modelling of semiconductor devices (lasers, transistors) in Orel State Technical University (Russia), in "Educational and Research Laboratory in Micro- and Nanoelectronics". In years 2013-2015 lectured at Rzeszów University, Rzeszów, Poland and researched on properties of nanoscale semiconductors at Teaching and Research Center of Microelectronics and Nanotechnology, in "Magnetotransport Laboratory for Low and Ultra-low Temperatures". Since 2016 dr Koziol works at the

National Centre for Nuclear Research, in Laboratory of Materials Research, performing Molecular Dynamics simulations of physical phenomena in materials under nuclear irradiation. His latest interests include investigation of properties of 2D materials like graphene, and dynamics of stress field penetration and dislocations in steel and other materials.