Skoltech
Skolkovo Institute of Science and Technology

When: October 3, 15:00-16:00
Where: Skoltech, TPOC-3 (blue bld.), room 408

COMPUTATIONAL MATERIALS SCIENCE SEMINAR:

# MULTISCALE QM/MM MODELING OF MATERIALS CHEMOMECHANICS


## Speaker:
## Petr Grigorev

**Warwick Centre for Predictive Modelling, School of Engineering, University of Warwick, Coventry, United Kingdom**


## ABSTRACT


Fracture and plasticity are the dominant failure processes underlying many materi-als reliability issues. They are also some of the most challenging multiscale modellingproblems, requiring both an accurate description of chemical processes occurring nearcrack tips or dislocation cores and the inclusion of much larger model systems. Theserequirements can be met simultaneously by combining quantum mechanical descriptionsof chemically active regions with classical atomistic models that capture the long-rangeelastic behaviour of the surrounding crystal matrix, using approaches such as the 'Learnon the Fly (LOTF) scheme. I will start with a review of the previous studies of frac-ture and continue with more detailed description of recent results on dislocation glide intungsten.In this study we use a hybrid musltiscale approach, namely quantum mechanics/molecularmechanics (QM/MM) [1], combining an accurate local QM description of the dislocationcore atoms with a classical model for the rest of the system. We apply a recently de-veloped QM/MM implementation of the virtual work principle [2] to compute energybarriers. The effect of H and He atoms in the material on the dislocation core structuretogether with the energetics of dislocations and impurities are investigated. The obtainedresults are analysed by comparison with pure DFT studies from literature [3, 4, 5] togetherwith machine learning based Gaussian Approximation Potential (GAP) model [5].



[1] N. Bernstein, J. R. Kermode, and G. Csányi, Rep. Prog. Phys. 72, 026501 (2009).
[2] T. Swinburne, J. R. Kermode, Phys. Rev. B. 96, 144102 (2017).
[3] L. Dezerald, D. Rodney, E. Clouet, L. Ventelon, F. Willaime, Nat. Commun. 7, 11695 (2016)
[4] A. Bakaev, P. Grigorev, D. Terentyev, A. Bakaeva, E. E. Zhurkin, Y. A. Mastrikov, Nucl.Fusion 57, 126040 (2017)
[5] W. Slachta, A. Bartók and G. Csányi, Phys. Rev. B. 90, 104108 (2014).


## BIOGRAPHY

In May 2012 I got my master degree in Physics from Peter the Great St.PetersburgPolytechnic University with specialisation in Experimental Nuclear Physics. The topic of thethesis was Molecular Dynamics simulations of sputtering of Al, Si and SiC surfaces.In November 2012 I started as a Ph.D. student shared between University of Ghent in Belgiumand University of Complutense in Spain, however I spent most of my time in Belgian NuclearResearch Center SCK CEN in Mol, Belgium. The topic of the thesis was multi-scale modelling ofretention of plasma components in tungsten under high flux plasma exposure. The study wasmainly done within sequential multi scale modelling paradigm using DFT, MD and Kinetic RateTheory. The defence tool place on 27th of April 2017 in Gent, Belgium.In may 2017 I joined Warwick Centre for Predictive Modelling at Iniversity of Warwick to workon development and applications of hybrid QM/MM approach. Which will be the main topic of mepresentation.

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