11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20–25, 2014, Barcelona, Spain

# MODELING SURFACE STRESSES AT THE NANOSCALE BY ADAPTIVE ATOMISTIC-CONTINUUM COUPLING

**B. Eidel**[1,2], **N. Prajapati**[3]

[1] Institute of Mechanics, Department of Mechanical Engineering, University of Siegen, bernhard.eidel@uni-siegen.de, http://www.mb.uni-siegen.de/nm/
[2] Institute of Mechanics, Faculty of Engineering, University of Duisburg-Essen, bernhard.eidel@uni-due.de, https://www.uni-due.de/mechanika/
[3] ICAMS, Univ. Bochum, nir543mech@googlemail.com, http://www.icams.de

**Key words:** *Quasicontinuum Method, Atomistic-Continuum Coupling, Surface Stress, Nanomechanics, Finite Element Methods.*

Surface stress has a strong impact on the effective mechanical stiffness of crystalline structures at the nanoscale. The size-dependency of elastic stiffness in e.g. nanowires is one among great many examples. Based on achievements of existing methods and open gaps in the state of the art, [3, 5], we discuss critical aspects for the modeling of surface stress for crystalline solids at the nanoscale. Benchmarking in Computational Mechanics has been pushing the development of novel methods towards accuracy and efficiency, see e.g. [5] for the field of concurrent atomistic-continuum (a-c) coupling. In a similar spirit we propose a simple but fully fledged performance benchmark for surface relaxation and stress. We show that the cluster-based Quasi-Continuum (CQC) method, [2], [4], obtains quantitative agreement with Molecular Dynamics/Statics for an unprecedented efficiency. Remarkably, and to our best knowledge for the first time among a-c coupling methods, the modeling does not only capture surface stress at smooth surfaces, but also at edges and vertices as the challenging "hot spots" of surface topologies where other methods are known to fail, [3]. Since the excellent performance of CQC is strongly related to the methodic feature of adaptivity we believe that adaptive methods enabling a "smooth" transition to fully atomistic resolution like e.g. the original QC version based on Cauchy-Born elasticity [1] may perform comparably well.

## REFERENCES

[1] E.B. Tadmor, M. Ortiz, and R. Phillips. Quasicontinuum analysis of defects in solids. *Philos. Mag. A*, Vol. **73**, 1529–1563, 1996.

[2] J. Knap and M. Ortiz. An analysis of the quasicontinuum method, *J. Mech. Phys. Solids*, Vol. **49**, 1899–1923, 2001.

[3] H.S. Park, P. Klein, and G. Wagner. A surface CauchyBorn model for nanoscale materials. *Int. J. Numer. Methods Eng.*, Vol. **68**, 1072–1095, 2006.

[4] B. Eidel and A. Stukowski. A variational formulation of the quasicontinuum method based on energy sampling in clusters. *J. Mech. Phys. Solids*, Vol. **57(1)**, 87–108, 2009.

[5] R.E. Miller and E.B. Tadmor. A unified framework and performance benchmark of fourteen multiscale atomistic/continuum coupling methods. *Model. Simul. Mater. Sci. Eng.*, Vol. **17**, 053001, 2009.