Nanomechanics

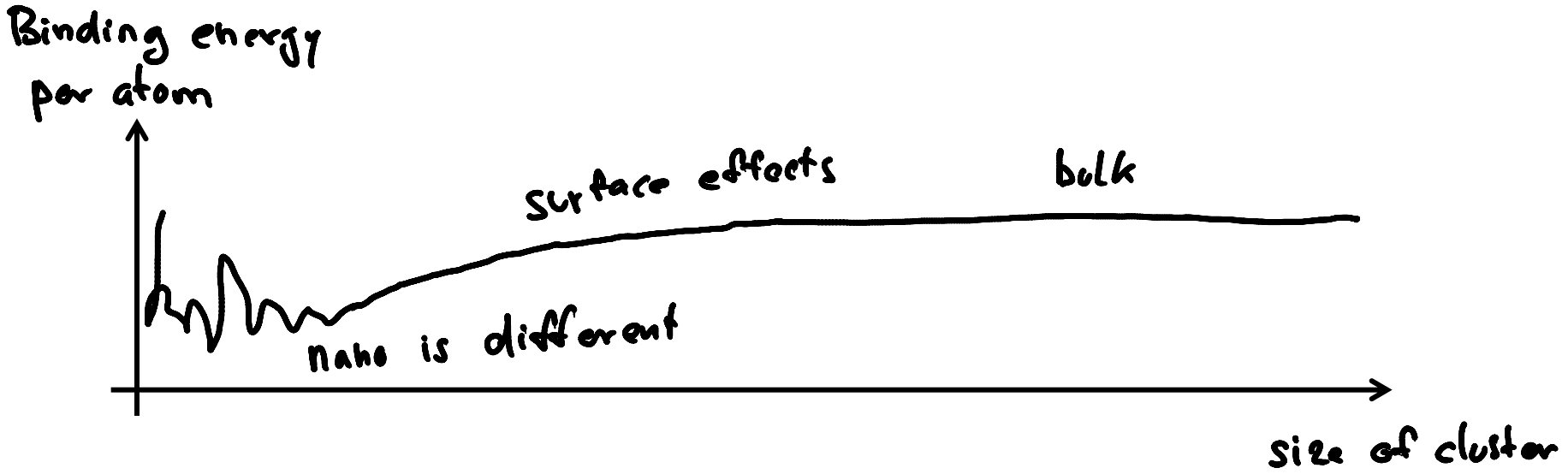
Introduction and lecture organization

What is Nanomechanics?

Mechanics – Science of forces and of kinetics

– Overlap with Quantum Mechanics and Statistical Mechanics

Nanoscience – Science of structures with dimensions on the nanometer scale



Quantum Mechanics and Statistical Mechanics

Nanometer $\hat{=}$ molecular Scale $\Rightarrow$ Quantum Mechanics

Energy scale $\hat{=}$ thermal energy $k_B T$

$\Rightarrow$ Statistical Mechanics is relevant

Example: Surface energy $50 \frac{mJ}{m^2}$

$$= \frac{0.05\ J}{1.6 \times 10^{-19} \frac{J}{eV}} \cdot \frac{1}{10^{18} nm^2} = 300 \frac{meV}{nm^2}$$

$k_B T = 26$ meV at room temperature

EU Definition of Nanomaterials

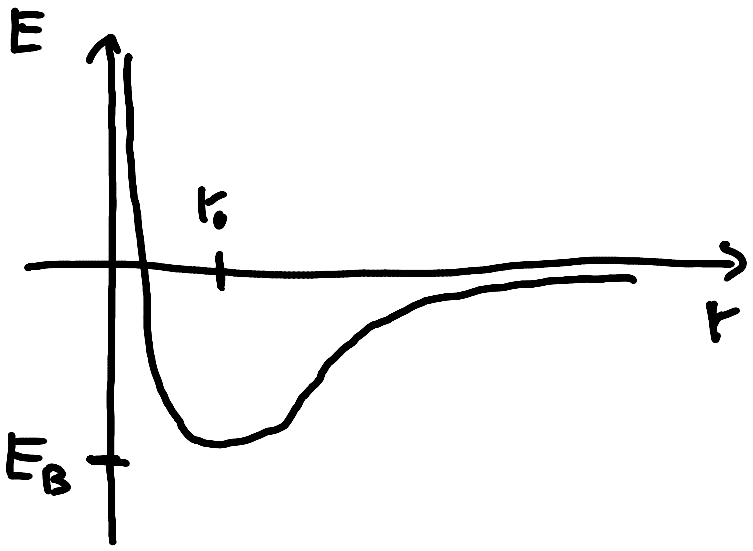
- On 18 October 2011 the Commission adopted the Recommendation on the definition of a nanomaterial. According to this Recommendation a "Nanomaterial" means:
- *A natural, incidental or manufactured material containing particles, in an unbound state or as an aggregate or as an agglomerate and where, for 50 % or more of the particles in the number size distribution, one or more external dimensions is in the size range 1 nm - 100 nm.*
- *In specific cases and where warranted by concerns for the environment, health, safety or competitiveness the number size distribution threshold of 50 % may be replaced by a threshold between 1 and 50 %.*
- *By derogation from the above, fullerenes, graphene flakes and single wall carbon nanotubes with one or more external dimensions below 1 nm should be considered as nanomaterials.*

Overview of lecture

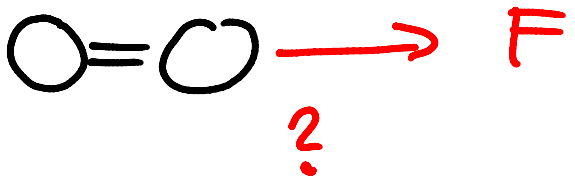
- Atomic interaction potentials and forces
- Molecular vibrations and spectroscopy
- Experimental methods of nanomechanics
- Molecular recognition by force measurements
- Force measurements on polymers
- Friction at the nanometer scale
- (Molecular dynamics simulations)

Atomic interaction potentials and forces

- Shape of potential, relation to macroscopic quantities, rate dependence of separation force



Van der Waals
ionic
covalent



Energy is a system parameter.

Nano => Forces can be measured

Towards time-dependent, non-equilibrium charge-transfer force fields

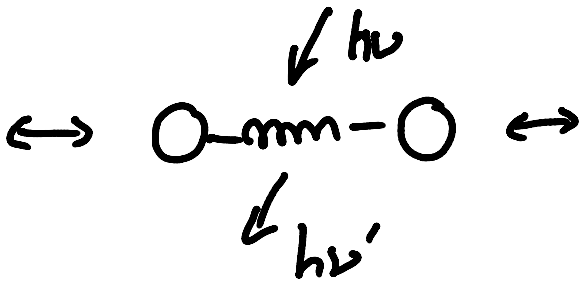
Contact electrification and history-dependent dissociation limits

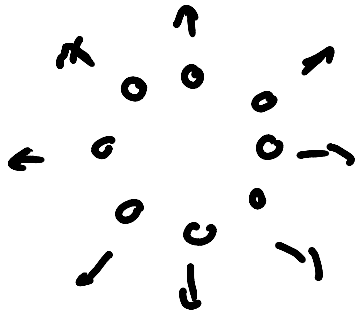
Wolf B. Dapp[1] and Martin H. Müser[1,2,a]

[1] Jülich Supercomputing Centre, Institute for Advanced Simulation, FZ Jülich, 52425 Jülich, Germany
[2] Department of Materials Science and Engineering, Universität des Saarlandes, 66123 Saarbrücken, Germany

Molecular vibrations and spectroscopy

- Infrared and Raman spectrsocopy, carbon nanotubes and graphene, isotope effects





$\nu = f(d)$

breathing mode

PHYSICAL REVIEW B **79**, 125442 (2009)

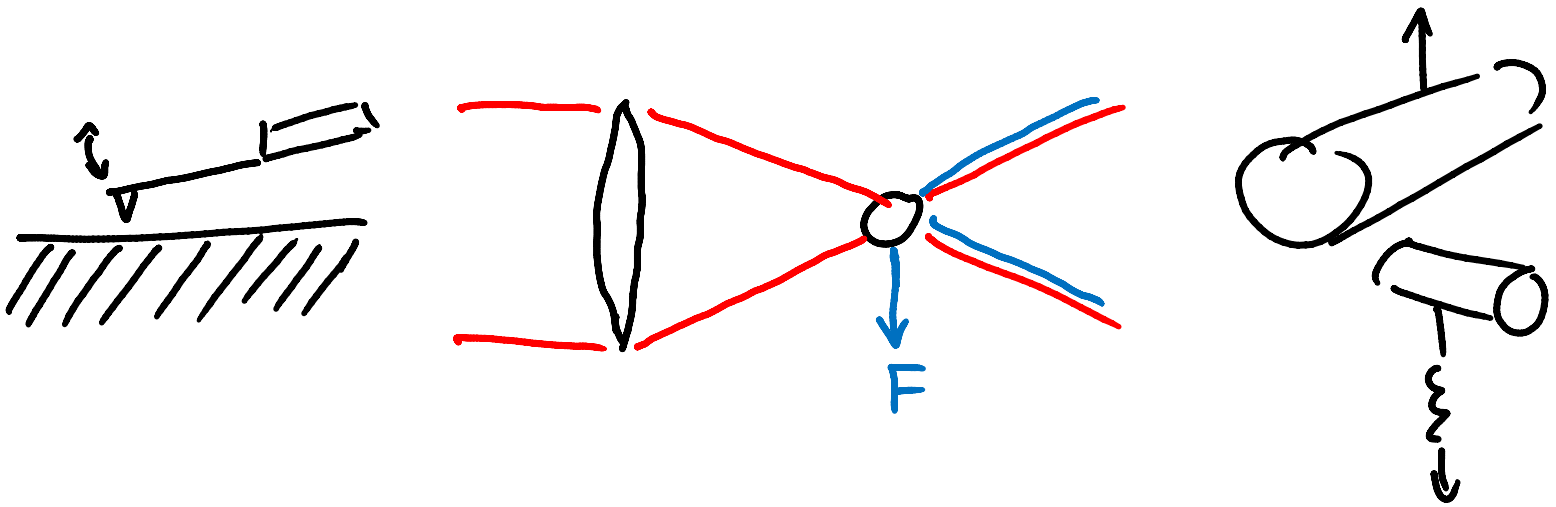
Phase transitions and molecular dynamics of *n*-hexadecanol confined in silicon nanochannels

R. Berwanger,[1] A. Henschel,[2] K. Knorr,[2] P. Huber,[2] and R. Pelster[1]
[1]*Universität des Saarlandes, FR 7.2 Experimentalphysik, 66041 Saarbrücken, Germany*
[2]*Universität des Saarlandes, FR 7.3 Technische Physik, 66041 Saarbrücken, Germany*
(Received 29 December 2008; revised manuscript received 12 February 2009; published 31 March 2009)

We present a combined x-ray diffraction and infrared spectroscopy study on the phase behavior and molecular dynamics of *n*-hexadecanol in its bulk state and confined in an array of aligned nanochannels of 8 nm diameter in mesoporous silicon. Under confinement, the transition temperatures between the liquid, the rotator

Experimental methods of nanomechanics

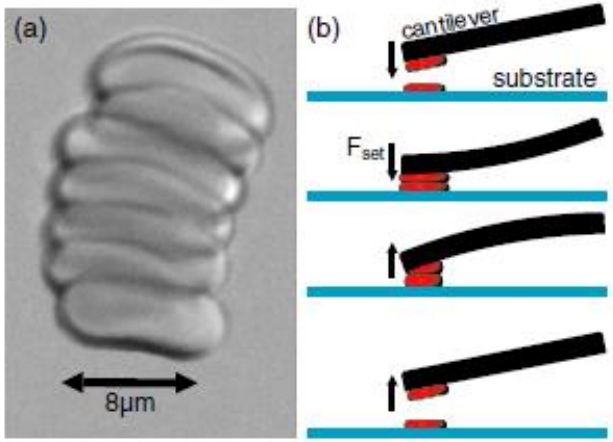
- AFM, optical and magnetic tweezer, surface forces apparatus



PRL 110, 018102 (2013) PHYSICAL REVIEW LETTERS week ending 4 JANUARY 2013

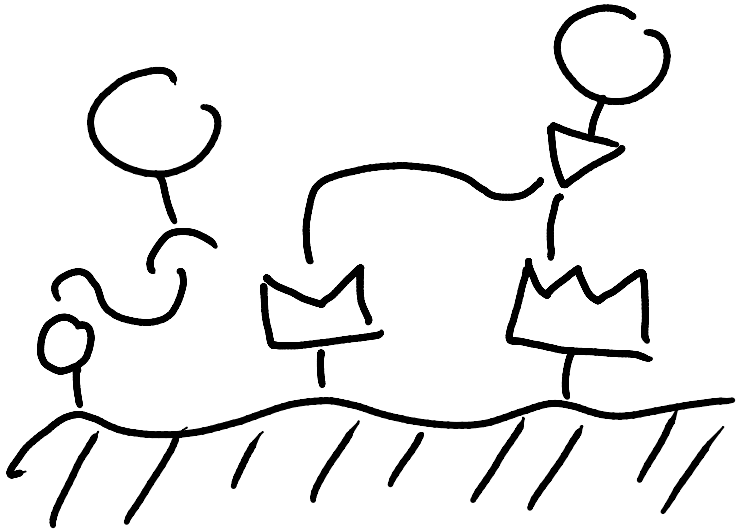
Quantification of Depletion-Induced Adhesion of Red Blood Cells

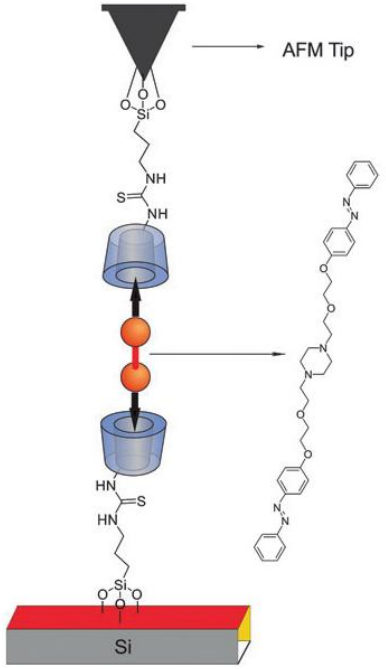
P. Steffen,[1] C. Verdier,[2] and C. Wagner[1]
[1]*Experimental Physics, Saarland University, 66041 Saarbrücken, Germany*
[2]*Laboratoire Interdisciplinaire de Physique (LIPhy), CNRS, Université de Grenoble I, UMR5588, 38041 Grenoble, France*
(Received 20 January 2012; published 2 January 2013)



Molecular recognition by force measurements

- Ligand-receptor interaction, antigen-antibody interaction, proteins and membranes





ChemComm

ROYAL SOCIETY OF CHEMISTRY

COMMUNICATION

Switching adhesion and friction by light using photosensitive guest–host interactions

Johanna Blass,[ab] Bianca L. Bozna,[a] Marcel Albrecht,[c] Jennifer A. Krings,[d] Bart Jan Ravoo,[d] Gerhard Wenz[c] and Roland Bennewitz*[ab]

CrossMark click for updates

Cite this: *Chem. Commun.*, 2015, 51, 1830

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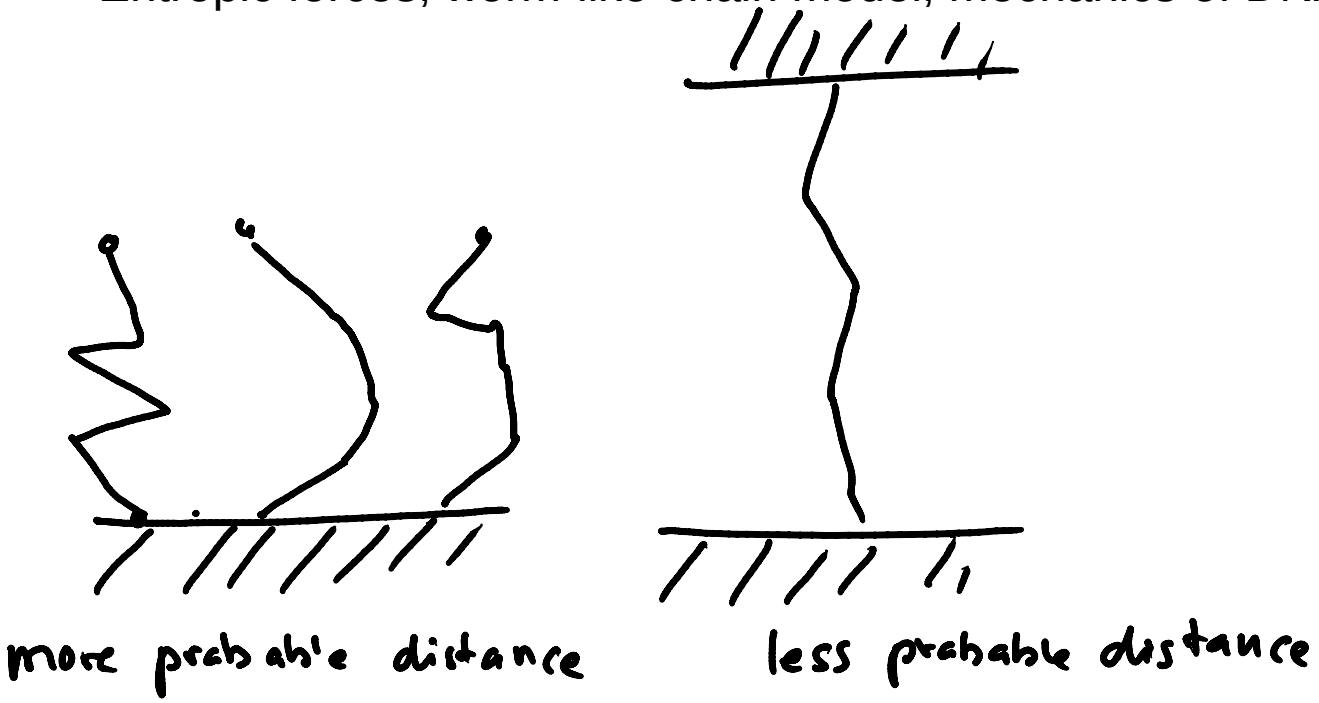
Accepted 11th December 2014

Force measurements on polymers

- Entropic forces, worm-like chain model, mechanics of DNA, protein folding



THE JOURNAL OF CHEMICAL PHYSICS **137**, 145105 (2012)

Coarse-grained Brownian dynamics simulations of protein translocation through nanopores

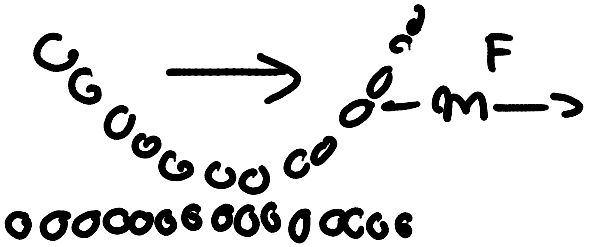
Po-Hsien Lee, Volkhard Helms, and Tihamér Geyer
Center for Bioinformatics, Saarland University, D-66041 Saarbrücken, Germany

(Received 17 July 2012; accepted 20 September 2012; published online 11 October 2012)

A crucial process in biological cells is the translocation of newly synthesized proteins across cell membranes via integral membrane protein pores termed translocons. Recent improved techniques

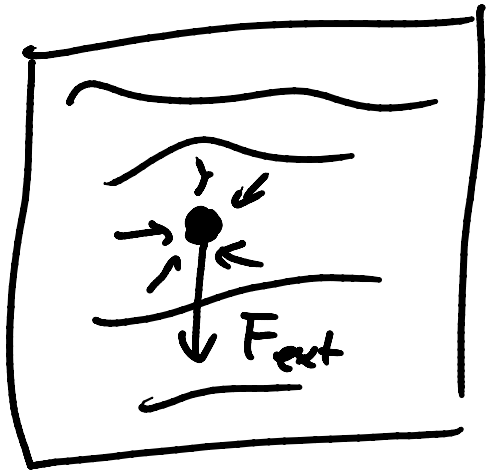
Friction at the nanometer scale

- Friction force microscopy, atomic friction phenomena, Tomlinson-Prandtl model, Langevin equation



Langevin – Equation

$$m \frac{dx^2}{dt^2} = -F_{ext} + F_f(t)$$



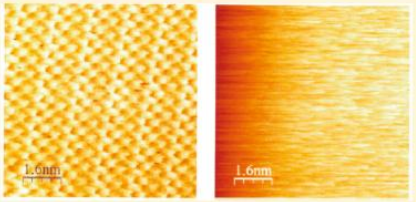
Molecular Order and Disorder in the Frictional Response of Alkanethiol Self-Assembled Monolayers

Nitya Nand Gosvami,[†,‡] Philip Egberts,[†] and Roland Bennewitz*[,†]

[†]INM—Leibniz Institute for New Materials, Campus D2 2, 66123, Saarbrücken, Germany

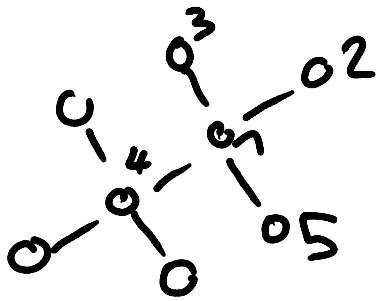
[‡]Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, United Kingdom

ABSTRACT: Molecular processes in the frictional response of an alkanethiol monolayer, self-assembled on a Au(111) surface, are studied by means of high-resolution friction force microscopy in ultrahigh vacuum. With increasing load, three regimes are observed on defect-free domains of the monolayer: smooth sliding with negligible friction, regular molecular stick–slip motion with increasing friction, and the onset of wear in the monolayer. Molecular contrast in the lateral force is found for inequivalent molecules within the unit cell of the c(4 × 2) superstructure. Significant differences in the frictional response are found between defect-free domains and areas including a domain boundary. Friction increases by an order of magnitude on domain boundaries in connection with irregular stick–slip motion. This increased friction at domain boundaries is observed at loads below the onset of wear.



Molecular dynamics simulations

- Fundamental of simulations, time scales, potentials, thermal equilibrium



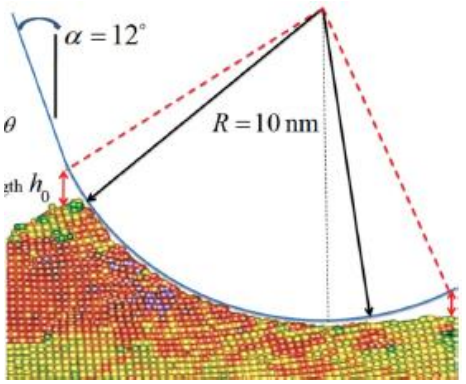
$$m_1 \ddot{x}_1 = -\sum \frac{dV(x_1 \ldots x_5)}{dx_1} + F(T, \dot{x}_1, \dot{x}_2)$$

PHYSICAL REVIEW B 86, 045452 (2012)

Friction model for single-asperity elastic-plastic contacts

Maneesh Mishra,[1] Philip Egberts,[2] Roland Bennewitz,[2,*] and Izabela Szlufarska[1,3,†]
[1]*Materials Science Program, University of Wisconsin–Madison, Madison, Wisconsin 53706, USA*
[2]*INM-Leibniz Institute for New Materials, Campus D2 2, 66123 Saarbrücken, Germany*
[3]*Department of Materials Science and Engineering, University of Wisconsin–Madison, Madison, Wisconsin 53706, USA*
(Received 12 April 2012; revised manuscript received 1 June 2012; published 30 July 2012)

In this article, we present an analytical model that describes the plowing coefficient of friction for sliding, elastic-plastic contacts between a conical tip with a spherical extremity and a flat substrate. The model includes the effects of adhesion and bridges the gap between models which are based solely on dislocation activity and those based solely on interfacial effects scaling with the contact area. The Derjaguin-Muller-Toporov approximation for adhesive contact stress is used in our description of the contacts. Our model shows excellent agreement with large-scale molecular dynamics simulations and atomic force microscopy experiments of nanoscratching on



Grading

- Credit points and grade will be given based on two components:
  - Test written in the last lecture of the semester (January 31, 2018)
  - Presentation of a nanomechanics research paper in the *Übungen* with written report
  - Details on requirements for a presentation and a written report will follow
- In order to be admitted to the written test, students have to solve 9 sets of problems and reach 50% of the points in these problems (*Prüfungsvorleistungen*).
- Alternative *Prüfungsvorleistung*: In a group of three, develop a numerical solution of entropic forces for a single molecule in the freely-jointed chain model.

Übungen

- *Übungen* will be a mix of discussion of lecture content, solving of problems, discussion of solutions, discussion of nurmerics project, and presentations by students.
- Please bring a calculator to the *Übungen*.
- Participation is mandatory, send me an email if you can not attend.

r.bennewitz@mx.uni-saarland.de

Books

- Uwe Hartmann
  Nanostrukturforschung und Nanotechnologie
  Oldenbourg Verlag, München 2012
- Atsuki Ikai
  Einführung in die Nanobiomechanik
  Wiley-VCH, Weinheim 2010
- Andrew N. Cleland
  Foundations of Nanomechanics
  Springer-Verlag Berlin 2003

Finis

- Monday 10:15 – 11:50 lecture
- Wednesday 8:25 – 9:10 lecture
- Wednesday 9:15 – 10:00 Übung