Appendix 1
Presentations without Paper

Concurrent and Sequential Multi-Scale Simulations of Friction and Contact Mechanics
M. Müser

Molecular Dynamics Simulations of the Mechanical Properties of Nanotube-Reinforced Composite Materials
M. Griebel

Nanotube and Nanocomposite Mechanics
H.D. Wagner

On Issues in Multi-Scale Modeling of Damage in Heterogeneous Solids
R. Talreja

Surface/Edge Induced Intrinsic Size-Dependent Properties of Nanowires
T-Y. Zhang, M. Luo and W.K. Cha

QM/MM Hybrid Simulation of Bio-Nanosystem Immobilization on Various Substrates
Y-P. Zhao, Z. Yang and J. Yin

Search for a Source of Cavitation in Plasticity of Crystalline Polymers
A. Galeski, A. Pawlak and A. Rozanski

Transforming Nanoparticles – Experiments and Modeling
F.D. Fischer and D. Vollath

Atomistic Description of Nanoisland Growth: Co on Single Crystal Cu Surfaces
L. Diekhöner, N.N. Negulyaev, V.S. Stepanyuk, P. Bruno, P. Wahl and K. Kern

Understanding Brittle Fracture in Nanostructured Silicon Carbide by Atomistic Simulations
L. Colombo

Deformation and Failure Modes of a Single Nanofiber
*C.T. Lim*

Multiscale Modeling of Interface Fracture
*A. Siddiq and S. Schmauder*

Molecular Simulations of Deformation, Flow and Physical Aging in Glassy Solids
*J. Rottler*
Appendix 2
Scientific Programme

Monday 19 May, 2008

K.Y. Volokh – Multiscale failure modeling: From atomic bonds to hyperelasticity with softening
R.K. Kalia, A. Nakano and P. Vashishta – Multimilion-to-bilion atom molecular dynamics simulations of deformation, fracture and nanoductility in silica glass
M. Müser – Concurrent and sequential multi-scale simulations of friction and contact mechanics
M. Griebel – Molecular dynamics simulations of the mechanical properties of nanotube-reinforced composite materials
H.D. Wagner – Nanotube and nanocomposite mechanics
Ł. Figiel, F.P.E. Dunne and C.P. Buckley – Multiscale modelling of layered silicate/PET nanocomposites during solid-state processing
R. Talreja – On issues in multi-scale modeling of damage in heterogeneous solids
K. Jolley and S.P.A. Gill – Modelling transient heat conduction at multiple length and time scales: A coupled non-equilibrium molecular dynamics/continuum approach
V.B.C. Tan, M. Deng, T.E. Tay and K.M. Lim – Multiscale modeling of amorphous materials with adaptivity
P.K. Valavala and G.M. Odegard – Thermodynamically-consistent multiscale constitutive modeling of glassy polymer materials
L.C. Zhang – Effective wall thickness of single-walled carbon nanotubes for multiscale analysis: the problems and a possible solution
T-Y. Zhang, M. Luo and W.K. Chan – Surface/edge induced intrinsic size-dependent properties of nanowires
R. Pyrz and B. Bochenek – Discrete-continuum transition in modelling nanomaterials

Tuesday 20 May, 2008

B. Palosz – Looking beyond limitations of diffraction methods of structural analysis of nanocrystalline materials
G. Winther – Multiscale modeling of mechanical anisotropy in deformed metals

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J.M. Hill – Geometry and mechanics of carbon nanotubes and gigahertz nanoooscillators

V.A. Eremeyev and H. Altenbach – On the eigenfrequencies of an ordered system of nano-objects

H.L. Duan, J. Weissmuller, Y. Wang and X. Yi – Monitoring of molecule absorption and stress evolutions by in situ microcantilever systems

Y-P. Zhao, Z. Yang and J. Yin – QM/MM hybrid simulation of bio-nanosystem immobilization on various substrates

E.R. Hernandez – Using thermal gradients for actuation at the nanoscale

O. Sigmund – Systematic design of nano-photonic crystals and meta-materials

J. Chen and S.J. Bull – Modelling of indentation and scratch damage in multilayer coatings and bulk materials

F.D. Fischer and D. Vollath – Transforming nanoparticles – experiments and modelling

L. Diekhöner, N.N. Negulyaev, V.S. Stepanyuk, P. Bruno, P. Wahl and K. Kern – Atomistic description of nanoisland growth: Co on single crystal Cu surfaces

Wednesday 21 May, 2008

L. Colombo – Understanding brittle fracture in nanostructured silicon carbide by atomistic simulations

I.N. Remediakis – Atomistic models for the mechanical response of nanomaterials

C.T. Lim – Deformation and failure modes of a single nanofiber

H.J. Chu, H.L. Duan, J. Wang and B.L. Karihaloo – Elastic fields in quantum dot structures with arbitrary shapes and interface effects

J. Yvonnet, H. Le Quang and Q.-C. He – Thermo-mechanical numerical modelling of nano-inclusions with arbitrary shapes

H.L. Duan, B.L. Karihaloo and J. Wang – Thermo-elastic size-dependent properties of nanocomposites with imperfect interfaces

R.J. Young, S. Cui, I. Kinloch, Ch.C. Kao, S. Eichhorn and P. Kannan – Modelling the stress transfer between carbon nanotubes and a polymer matrix

A. Siddiq and S. Schmauder – Multiscale modeling of interface fracture

P. Olsson, C. Persson and S. Melin-Petersson – A study of the elastic properties of iron nanowires

T. Burczynski, W. Kus and A. Mrozek – Advanced continuum-atomistic model of materials based on coupled boundary element and molecular approaches

J.Y.H. Chia – Finite element modeling nanocomposites and interface effects on mechanical properties

I. Goldhirsch – Small scale and/or high resolution elasticity

M. Fermeglia – Enthalpic and entropic effects of nanoparticles in polymer matrices: Industrial applications
Thursday 22 May, 2008

O.B. Naimark – Structural-scaling transitions in mesodefect ensembles and properties of bulk nanostructural materials – Modeling and experimental study

J. Rottler – Molecular simulations of deformation, flow and physical aging in glassy solids

T.A. Kowalewski, S. Barral and T. Kowalczyk – Modeling electrospinning of nanofibres

J. Jancar – Use of reptation dynamics in modeling molecular interphase in polymer nanocomposite

A. Rozanski, A. Galeski and J. Golebiewski – Low density polyethylene-montmorillonite nanocomposites for film blowing
Appendix 3
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Crack Initiation, Kinkind and Nanoscale Damage in Silica Glass: Multimillion-Atom Molecular Dynamics Simulation


Fig. 1 Nucleation of nanocavities and crack nanocolumns in a tensile-stress region around the pre-crack tip. The inset shows the setup of the simulation. The white rectangular plate is a rigid indenter, the light blue parallelepiped is the silica glass of dimensions 120 × 120 × 15 nm$^3$, and the dark blue region denotes a pre-crack of length 40 nm and width 15 nm. Dotted line indicates the direction along which the nanocavities nucleate. Damage nanocavities (red, orange, yellow, green) and nanocolumns (blue) in the tensile stress region. The impact loading speed is 0.05$v_R$, where $v_R$ is the Rayleigh wave speed.
Fig. 2 Formation of a wing crack via growth and coalescence of nano-columns and nanocavities at an impact loading speed of $0.05v_R$. (a) A snapshot taken after 19 ps shows cavities (red, orange, yellow, green and dark blue) around nanocolumns (blue). (b) In the next couple of picoseconds, nanocolumns merge and coalesce with nanocavities to form a wing crack.

Fig. 3 Second healing of the wing crack at the loading speed of $0.05v_R$. (Right) A snapshot of the wing and primary cracks (blue) just after healing begins. The wing-crack tip is split up into two nanocolumns and there are a few damage cavities (green and red) near the tip. (Middle) In 4 ps the wing crack has receded considerably and left several cavities (red, yellow, green and blue). (Left) A snapshot of the wing crack and cavities after the crack stops healing. The residual length of the wing crack is slightly less than half of the maximum length.
Multiscale Modelling of Layered-Silicate/PET Nanocomposites during Solid-State Processing

Fig. 1 Simulated stress-strain curves – effect of silicate loading; $T = 95^\circ$C.

Fig. 2 Simulated deformation and contour plots representing onset of crystallization at applied strains: (A) 0.5, (B) 1; temperature: 95$^\circ$C; applied strain rate: $1 \text{s}^{-1}$; legend: 1 – lock-up of viscous flow due to crystallization at all integration points of a finite element, 0 – no lock-up.
Fig. 3 Strain amplification factor at different volume fractions; $T = 95^\circ$C; applied strain rate: $1 \text{ s}^{-1}$.

Fig. 4 Effect of processing temperature on the nanocomposite morphology; (A) $T = 100^\circ$C, (B) $T = 110^\circ$C; strain rate: $1 \text{ s}^{-1}$. 
Multiscale Modeling of Amorphous Materials with Adaptivity

Fig. 1 Strain contours from multiscale simulation just before crack propagation.

Fig. 2 Strain contours at the end of multiscale simulation.
Thermodynamically-Consistent Multiscale Constitutive Modeling of Glassy Polymer Materials

Fig. 1 Molecular RVEs of two polymer systems.

Polyimide
Polycarbonate
Discrete-Continuum Transition in Modelling Nanomaterials

Fig. 4 Non-homogeneity measure for three shear deformation levels of the diamond sheet.

Fig. 5 Non-homogeneity measure for the real structure and the structure deformed in an affine manner (a); colour code slip vector module that indicates displacement difference between non-affine (real) and affine displacement field (b).
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Fig. 9 Colour code atomic tensile strain components at different deformation levels.
Multiscale Modelling of Mechanical Anisotropy of Metals
*G. Winther*, pp. 89–98.

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**Fig. 3** Typical bilayer periodic microstructure and Finite Element mesh used for generating full-field reference solutions. The top and thick layer is soft and made of anisotropic grains (“Cu-like” behaviour). The thin bottom layer is made of isotropic W grains.
Fig. 4 Distribution of equivalent elastic strain in (top) the soft “Cu-like” layer, and (bottom) the stiff W layer. The applied macroscopic axial stress is 100 MPa. Results generated for $a = 100$. Note the different color scales for both figures.
Monitoring of Molecule Adsorption and Stress Evolutions by In-Situ Microcantilever Systems
H.L. Duan, Y. Wang and X. Yi, pp. 133–140.

Fig. 4 Variation of curvature $\kappa$ with island coverage $q$ and island size $L$ ($\varphi = 10^\circ$, $t_f = 1.4$ nm, $t_s = 0.5$ $\mu$m).

Using Thermal Gradients for Actuation in the Nanoscale

Fig. 1 Schematic picture of the mobile element of the nanofabricated device. The long inner nanotube (shown in yellow) is suspended between the two electrodes; the gold platelet is attached to the outer nanotube (shown in red), which can slide down and rotate around the inner nanotube due to the low friction contact between nanotube walls.
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Systematic Design of Metamaterials by Topology Optimization
O. Sigmund, pp. 151–159.

Fig. 1 The inverse homogenization problem. White arrows indicate the conventional forward homogenization approach, and black arrow indicate the inverse homogenization approach.
Fig. 3 Left: Topology optimized negative Poisson’s ratio materials (from [12]). Right: Topology optimized negative thermal expansion material (from [21, 22]).

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Thermo-Elastic Size-Dependent Properties of Nano-Composites with Imperfect Interfaces
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Modeling the Stress Transfer between Carbon Nanotubes and a Polymer Matrix during Cyclic Deformation
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Modeling Electrospinning of Nanofibers

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