

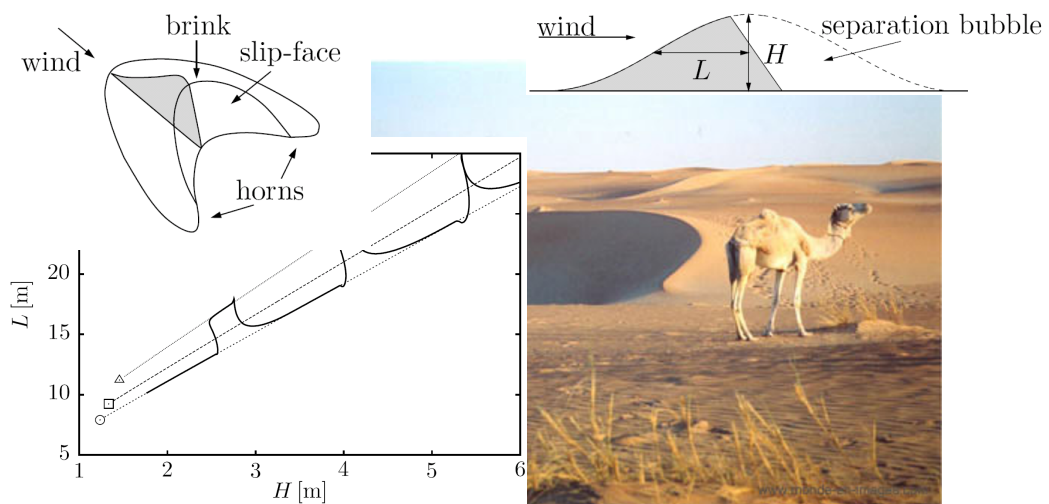
Jahresbericht 2006

Progress Report 2006

GRUPPE THEORIE WEICHER MATERIE
SOFT MATTER THEORY GROUP

Abteilung Theorie kondensierter Materie
Condensed Matter Theory Section

Institut für Theoretische Physik
Universität Leipzig



Cover picture: Characteristic for barchan dunes is their crescent shape with a lee-facing slip zone. The central cross-sections of differently sized dunes has been found to be rescalable onto a master curve introducing typical length scales H and L . The graph in the lower left corner shows L vs. H as the wind strength fluctuates.

Das Jahr 2006

The year 2006

In 2006, we achieved good progress in various fields of soft condensed matter theory: From cell mechanics over polymer networks to the dynamics of a single semi-flexible polymer, and the jamming transition of colloidal suspensions.

Our group greatly welcomed Dr. Pablo Fernandez as long-term guest with his expertise on viscoelasticity which he brought forward in his winter term lecture. Another highlight was graduate Benedikt Obermayer being awarded the “Physik-Studienpreis der Wilhelm und Else Heraeus-Stiftung”.

In the course of the year, Jens Glaser and Daniel Rings both finished their diploma theses with success, and a new student, Sebastian Schöbl, joined our group.

Klaus Kroy

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1 Gruppenstruktur

Group structure

1.1 Mitarbeiter

Members

- Prof. Dr. Klaus Kroy,
Universität Leipzig, ITP-1R14, Tel. 0341 9732436
- Benedikt Obermayer,
Universität Leipzig, Linnéstr. 5 - 487, Tel. 0341 9732610
- Jens Glaser,
Universität Leipzig, Linnéstr. 5 - 487, Tel. 0341 9732610
- Daniel Rings,
Universität Leipzig, Linnéstr. 5 - 487, Tel. 0341 9732610
- Steffen Arnrich,
Universität Leipzig, Linnéstr. 5 - 487, Tel. 0341 9732610
- Sebastian Schöbl,
Universität Leipzig, Linnéstr. 5 - 487, Tel. 0341 9732610

1.2 Gastwissenschaftler

Longterm Guest

- Dr. Pablo Fernandez,
Universität Bayreuth, Lehrstuhl Experimentalphysik I,
95440 Bayreuth, Tel. 0921 55 2502

2 Projekte

Projects

2.1 Biopolymers

Benedikt Obermayer, Jens Glaser, Klaus Kroy

Many important biopolymers are accurately described by the wormlike chain model. With this model, the dynamic structure factor for a single chain is being studied revealing information about the thermal fluctuations of the polymer in a solvent. Hydrodynamic interactions needed to be taken into account in order to obtain consistent results. Another investigation resulted in a unified picture of the effects of a stretching force applied at the ends of such an inextensible chain. A concise explanation of the dominant relaxation mechanisms has been given and a full characterization of the dynamic longitudinal response of stiff polymers and stretched (semi)flexible filaments has been developed: (i) a straight initial configuration due to strong stretching is not equivalent to an initial low-temperature environment (quenching); (ii) monitoring eigenvalues of the gyration tensor is not equivalent to measuring the actual end-to-end distance.

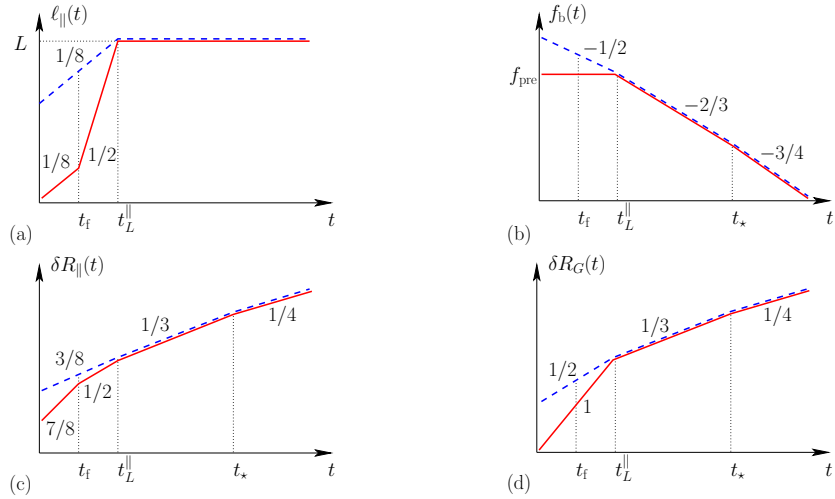


Figure 1: Stretching (solid) vs. quenching (dashed). Asymptotic scaling laws for the boundary layer size $l_{par}(t)$ (a), for the bulk tension $f_b(t)$ (b), for the change in end-to-end distance $\delta R_{||}(t)$ (c), and for the change in the gyration tensor's eigenvalue $\delta R_G(t)$ (d) vs. time t (log-log scale). The stretching force f_{pre} has been related to the quenching strength $r = \ell_p^</>/\ell_p^>$ via $f_{pre} = r^4 \kappa (\ell_p^>/L^2)^2$.

2.2 Cell Mechanics

Pablo Fernandez, Klaus Kroy

Unlike the concrete and steel of buildings and bridges, most mechanical elements of biological cells are soft, in that their shape is subject to significant thermal fluctuations. The cytoskeleton provides mechanical stability and integrity of biological cells. In close cooperation with experimentalist Andreas Bausch, the biological complexity has been reviewed from a physicist's perspective.

Figure 2: Fluorescent micrographs of emulsion droplets containing rhodamine phalloidin-labelled actin filaments. In small droplets ($D < 12$ microns), the actin is organized in a cortex close to the droplet surface (I), whereas it is more homogeneously distributed in large droplets (II). The scale bar is 10 microns. In general, actin solutions encapsulated in sufficiently small emulsion droplets are locally more heterogeneous and more elastic than bulk solutions.

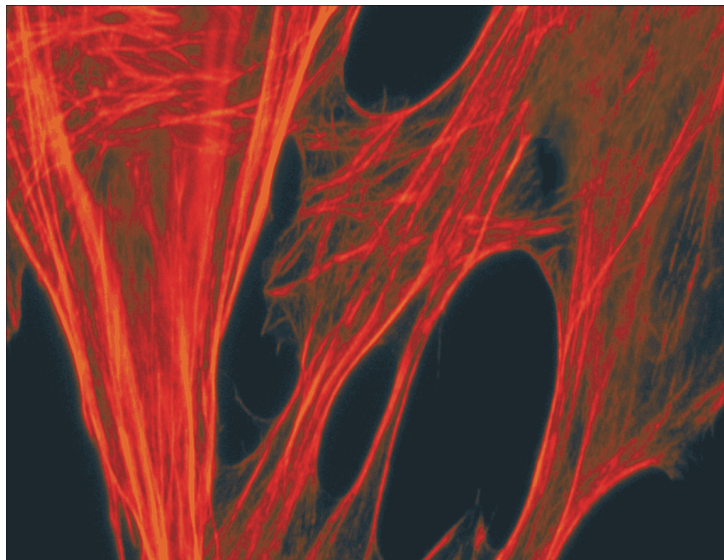
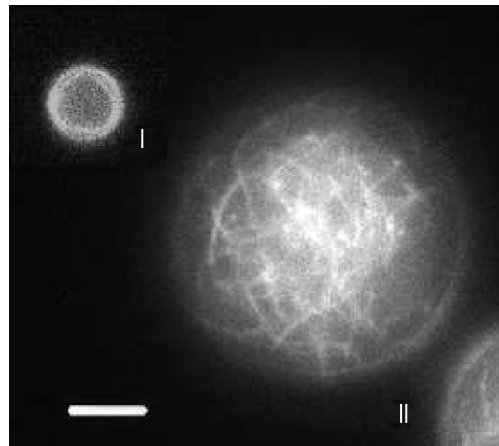


Figure 3: Microscopic image of a cell's (dyed) cytoskeleton. Filament bundles are clearly recognized as well as interconnecting crossings.

2.3 Colloidal Aggregation

Daniel Rings, Klaus Kroy

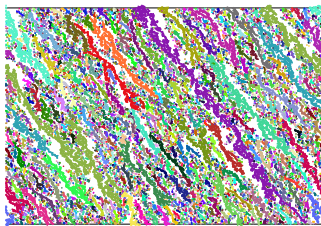
Describing particle coagulation is of great interest in various branches of research from medicine to engineering. Shear-induced gelation, i. e. the transition from sol to gel, is accompanied by a sharp increase in viscosity which may pose considerable problems both in technological as well as life sciences.

Our numerical study of a two-dimensional toy model for the phenomenon of shear-driven aggregation and gelation in suspensions of adhesive colloids has two objectives:

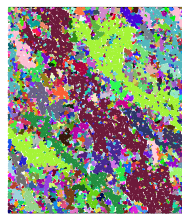
- to develop an efficient simulation algorithm
- to analyze the most salient features of shear-driven aggregation that distinguish it from other common kinetic models such as diffusion- or reaction-limited cluster aggregation, as well as the crossover to universal percolation behavior at gelation.



(a) $\phi = 0.1$



(b) $\phi = 0.2$



(c) $\phi = 0.4$

Figure 4: Snapshots of spanning clusters in the final state of simulations at different area fractions. At low densities the clusters have rather isotropic shapes, and their orientation is not clear. Around $\phi = 0.2$, a stringy shape is most pronounced and orientational alignment is strong, while at high ϕ it weakens again, and clusters become "fatter".

2.4 Sand dunes

Sebastian Fischer, Klaus Kroy

In collaboration with H. Herrmann of the University of Stuttgart a minimal model has been formulated which elucidates the basic physical mechanisms underlying dune formation and migration. It allows us to analyze the effect of environmental conditions uncontrollable in the field on the characteristic shapes of dunes systematically. While the previously studied stationary solutions obtained under periodic boundary conditions are "unphysical" in the sense that they correspond to unstable fixed points of the equations, the solutions for open boundary conditions are shown to be strongly constrained by the unstable manifolds of these fixed points.

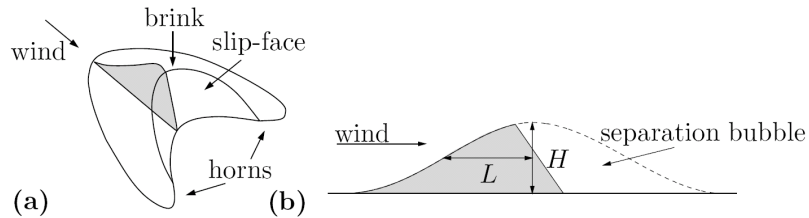


Figure 5: (a) Sketch of a barchan dune. (b) Central slice of a barchan dune. Beyond the brink, inside of the so-called separation bubble the air flow near the ground is stagnant or even reverse. As a consequence, there is no wind erosion on the slip face. The height profile can be parameterized by height H and windward length L at half height of the common envelope of the dune profile and its separation bubble.

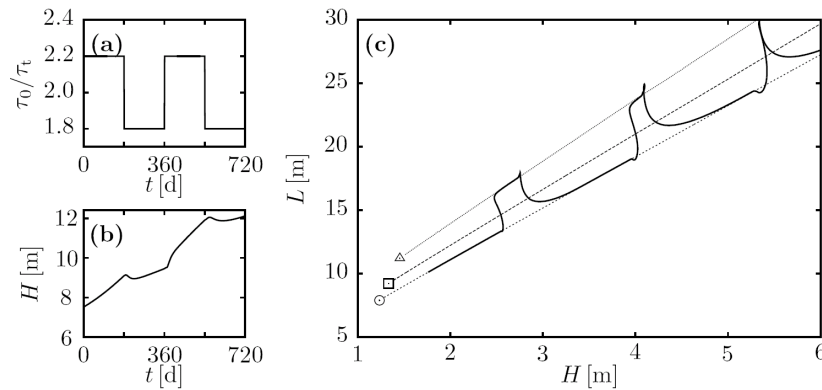


Figure 6: Evolution of a growing dune subject to periodically changing wind strength. (a) Shear stress protocol. (b) Evolution of the height H . (c) Reduced phase space trajectory of a growing heap recorded for three cycles (solid line). As long as the dune volume is small, the trajectory switches rapidly between the unstable manifolds with $\tau_0/\tau_t = 1.8$ (triangle) and $\tau_0/\tau_t = 2.2$ (circle).

3 Veröffentlichungen

Publications

Microrheology Probes Length Scale Dependent Rheology

J. Liu, M. L. Gardel, K. Kroy, E. Frey, B. D. Hoffman, J. C. Crocker, A. R. Bausch, and D. A. Weitz

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⁵ Physik-Dept E22, Technische Universität München, D-85748 Garching, Germany

Phys. Rev. Lett. 96, 118104 (2006)

We exploit the power of microrheology to measure the viscoelasticity of entangled F-actin solutions at different length scales from 1 to 100 μm over a wide frequency range. We compare the behavior of single probe-particle motion to that of the correlated motion of two particles. By varying the average length of the filaments, we identify fluctuations that dissipate diffusively over the filament length. These provide an important relaxation mechanism of the elasticity between 0.1 and 30 rad/sec.

Microstructure and viscoelasticity of confined semiflexible polymer networks

M. M. A. E. Claessens¹, R. Tharmann¹, K. Kroy, A. R. Bausch¹

¹ E22-Biophysics, Technische Universität München, James Franck Straße, 85748 Garching, Germany

Nature Physics 2, 186 - 189 (01 Mar 2006) Letters

The rapidly decreasing dimensions of many technological devices have spurred interest in confinement effects. Long before, living organisms invented ingenious ways to cope with the requirement of space-saving designs down to the cellular level. Typical length scales in cells range from nanometres to micrometres so that the polymeric constituents of the cytoskeleton are often geometrically confined. Hence, the mechanical response of polymers to external confinement has potential implications both for technology and for our understanding of biological systems alike. Here we report a study of *in vitro* polymerized filamentous actin confined to emulsion droplets. We correlate observations of the microstructure, local rheological properties and single-filament fluctuations. Enforcing progressively narrower confinement is found to induce a reduction of polymer fluctuations, network stiffening, structural heterogeneities and eventually cortex formation. We argue that

the structural and mechanical effects can be consistently explained by a gradual suppression of single-polymer eigenmodes.

Binding of TmHU to single dsDNA as observed by optical tweezers

M. Salomo, K. Kroy, K. Kegler, C. Gutsche, M. Struhalla, J. Reinmuth, W. Skokov, C. Imisch, U. Hahn, F. Kremer

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J Mol Biol. 2006 Jun 9;359(3):769-76. Epub 2006 Apr 19

Optical tweezers are employed to study the action of the histone-like protein from *Thermotoga maritima* (TmHU) on DNA at a single molecule level. Binding and disruption of TmHU to and from DNA are found to take place in discrete steps of 4-5 nm length and a net binding enthalpy of about $16k_B T$. This is in reasonable agreement with a microscopic model that estimates the extension of the binding sites of the protein and evaluates the energetics mainly for bending of the DNA in the course of interaction.

A bottom-up approach to cell mechanics

A. R. Bausch¹, K. Kroy

¹ E22-Biophysics, Technische Universität München, James Franck Straße, 85748 Garching, Germany

Nature Physics 2, 231 - 238 (01 Apr 2006)

The mechanical stability and integrity of biological cells is provided by the cytoskeleton, a semidilute meshwork of biopolymers. Recent research has underscored its role as a dynamic, multifunctional muscle, whose passive and active mechanical performance is highly heterogeneous in space and time and intimately linked to many biological functions, such that it may serve as a sensitive indicator for the health or developmental state of the cell. *In vitro* reconstitution of 'functional modules' of the cytoskeleton is now seen as a way of balancing the mutually conflicting demands for simplicity, which is required for systematic and quantitative studies, and for a sufficient degree of complexity that allows a faithful representation of biological functions. This bottom-up strategy, aimed at unravelling biological complexity from its physical basis, builds on the latest advances in technology, experimental design and theoretical modelling, which are reviewed in this progress report.

Elasticity, dynamics and relaxation in biopolymer networks

K. Kroy

Current opinion in colloid & interface science, vol. 11, no1 (2006), pp. 56-64

Our cells, muscles, and connective tissue owe their remarkable mechanical properties to biopolymer networks. Their incessant assembly, disassembly, restructuring, and active and passive mechanical deformation underlies the astounding robustness, adaptability, physical strength and motility of cells and of biological tissue in general. Unlike the flexible polymer networks discussed in standard texts on polymer physics, most biological macromolecular assemblies are predominantly made from (mixtures of) stiff polymers, however. The resulting local mechanical anisotropy and persistence entail distinct mechanical and dynamic properties unlike those familiar from synthetic polymers, foams, or other cellular structures. At the same time they pose formidable difficulties to theoretical modeling efforts, which were so far unsuccessful in establishing a generally accepted view of the origin of the macroscopic elasticity and equilibrium dynamics, let alone the complex biological function of biopolymer networks.

Dynamics of Aeolian Sand Heaps and Dunes: The Influence of the Wind Strength

S. Fischer & K. Kroy

in Traffic and Granular Flow '05, A. Schadschneider *et al.* (eds.), Springer, Heidelberg (2007).

The so-called *minimal model* provides an efficient minimum mathematical description of aeolian sand dune formation based on turbulent boundary layer calculations and a mean-field like saltation model. It allows us to analyze the effect of environmental conditions – uncontrollable in the field – on the characteristic shapes of dunes systematically. While the previously studied stationary solutions obtained under periodic boundary conditions are “unphysical” in the sense that they correspond to unstable fixed points of the equations, the solutions for open boundary conditions are shown to be strongly constrained by the unstable manifolds of these fixed points. For morphological evolution under periodically (e.g. seasonally) changing wind conditions a rule of thumb emerges, saying that the shapes of comparatively small/large dunes are slaved by the unstable manifolds pertaining to the actual/time-averaged environmental conditions, respectively.

4 Vorträge und Poster auf Konferenzen und Tagungen

Talks and Posters at Conferences and Workshops

- 31st Conference of the Middle European Cooperation in Statistical Physics 23-26 April 2006, Primosten, Croatia
Klaus Kroy: *How does a stretched polymer relax?*
- DPG-Meeting, 27-31 March 2006, Dresden
Benedikt Obermayer: *Dynamics of single semiflexible polymers under force*
Jens Glaser: *Hydrodynamic interactions for stiff polymers*
Daniel Rings: *Shear-driven gelation in two dimensions* (poster)
- 7th NTZ-Workshop on Computational Physics, 30 November - 02 December 2006, Universität Leipzig
Daniel Rings: *Simulation of shear-driven aggregation*

5 Gastvorträge an wissenschaftlichen Einrichtungen

Invited Talks at Academic Institutions

- Martin-Luther-Universität Halle-Wittenberg
Klaus Kroy: *Tension Dynamics in Stiff Polymers*
- Otto von Guericke Universität, Magdeburg
Klaus Kroy: *On Growth and Form of Desert Dunes*

6 Sonstiges

Miscellaneous

- Leipziger Buchmesse
Klaus Kroy: *Warum ist die Wüste nicht flach? Und warum ist das mathematisch so schwer zu beweisen?*

7 Vorlesungen

Lectures

7.1 SOSE 2006

Statistische Mechanik (Teil II)

Kursvorlesung, Universität Leipzig

Die Vorlesung gibt eine Einführung in theoretische Methoden zur Behandlung (überwiegend klassischer) wechselwirkender Vielteilchensysteme. Zunächst werden diskontinuierliche bzw. kontinuierliche Phasenübergänge im Rahmen der "Variational-mean-field-theory", Dichtefunktionaltheorie bzw. der Renormierungsgruppe diskutiert. Ein zweiter Teil wird der Brownschen Dynamik und der dynamischen Formulierung des Fluktuations-Dissipations-Theorems gewidmet sein.

Zur Abrundung soll abschließend ein schlaglichtartiger Ausblick auf aktuelle Forschungsschwerpunkte in der Statistischen Mechanik (Nichtgleichgewicht, Unordnung, Glasdynamik, Fluktuationstheoreme...) gegeben werden.

7.2 WISE 2006/2007

Quantenmechanik (Lehramt)

Kursvorlesung, Universität Leipzig

Die Vorlesung bietet eine Einführung in die Grundelemente der Quantenmechanik. Ausgehend von der klassischen Mechanik wird die Schrödinger-Gleichung motiviert und der übliche Formalismus der Operatordarstellung in Impuls- und Ortsraum eingeführt. Problemstellungen wie Potentialtöpfe, harmonischer Oszillator und Wasserstoffatom werden diskutiert und in Hausübungen vertieft.

Nichtgleichgewichtsphysik von Biopolymeren und molekularen Motoren

Wahlfach, Vorlesung, Universität Leipzig

Die Vorlesung ist unterschiedlichen aktuellen Themen der Nichtgleichgewichtsphysik weicher Materie gewidmet. Weiche Materie ist strukturell meist durch stark fluktuierende mesoskalige Strukturen (Kolloide, Polymere, Membranen, Proteine etc.) charakterisiert, deren statistische Konformation und stochastische Dynamik von Interesse sind. Maßgebliche theoretische Konzepte sollen anhand von paradigmatischen Modellen eingeführt werden. Themenvorschläge:

Wie es bei molekularen Motoren zum Verkehrsstau kommt (TASEP); Wie das Gleichgewicht die Nichtgleichgewichtsfluktuationen in Schach hält (Fluktuationstheoreme); Was passiert, wenn ein gestrecktes DNA-Molekül zerreißt (Nichtgleichgewichtsdynamik von Polymeren).

Nichtlineare Elastizität und Viskoplastizität lebender Materie

Ergänzungsveranstaltung mit Dr. Pablo Fernandez, Vorlesung, Universität Leipzig

Die Vorlesung bietet eine Einführung in die Biomechanik. Im ersten Teil werden die Grundlagen der Kontinuumsmechanik behandelt. Beispielfhaft werden Stoffgesetze dargestellt, mit denen die mechanischen Eigenschaften biologischer Systemen erfolgreich beschrieben werden können: Hyperelastizität, lineare Viskoelastizität, Viskoplastizität. Der zweite Teil der Vorlesung ist bestimmten biologischen Systemen gewidmet. Die mechanischen Eigenschaften von Geweben, einzelnen Zellen und dem Zytoskelett werden dargestellt. Schließlich wird ein Überblick über die aktuellen Fragen der Biomechanik gegeben.

8 Diplomarbeiten

Diploma theses

- Jens Glaser
“Dynamic Light Scattering of Stiff Polymers”
02/2006
- Daniel Rings
“Shear-Driven Aggregation: An Event-Driven Simulation Approach”
08/2006

9 Laufende Doktorarbeiten

PhD Theses in Progress

- Jens Glaser
“Strukturuntersuchung von F-Aktin-Lösungen: In der Arbeit geht es um die Theorie der dynamischen Lichtstreuung an semiflexiblen Polymeren sowie kollektive Effekte von Lösungen semiflexibler Polymere”
- Daniel Rings
“Dynamik granularer Medien im Strömungsfeld und Strukturbildung:

Ausgehend von einer Beschreibung des Transportmechanismus von Medien wie z.B. Sand in turbulenter Strömung werden verschiedene Strukturen - Dünen, Rippel, Kaustiken - und ihre Dynamik untersucht”

10 Preise

Awards

- Benedikt Obermayer
Physik-Studienpreis der Wilhelm und Else Heraeus-Stiftung
WS 2005/06

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