Metal and Material Physics Division Fachverband Metall- und Materialphysik (MM)

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Overview of Invited Talks and Sessions

(Lecture Rooms H4, H24, H25 and H26; Poster E)

Invited Talks

MM 1.1	Mon	9:30–10:00	H24	New opportunities and challenges in chromatic aberration corrected and in situ transmission electron microscopy — •RAFAL E. DUNIN- BORKOWSKI, LOTHAR HOUBEN, JURI BARTHEL, ANDREAS THUST, CHRIS BOOTHROYD, MARTINA LUYSBERG, ANDRAS KOVACS, MARTIAL DUCHAMP, JOACHIM MAYER
MM 6.1	Mon	11:45-12:15	H4	Prospects for mapping spins with atomic resolution in TEM $- \bullet$ JOHAN VERBEECK
MM 6.2	Mon	12:15-12:45	H4	Structural Characterization of nc-Si / SiO _x based quantum super- structures for the solar cell application by aberration-corrected high resolution electron microscopy — •MARYAM BEIG MOHAMADI, BIRGER BERGHOFF, JOACHIM MAYER
MM 10.1	Mon	15:00-15:30	H24	Materials Science and Development of Complex Materials — •JAN SCHROERS
MM 16.1	Tue	9:30-10:00	H24	Combinatorial approach to multifunctional materials — •ICHIRO TAKEUCHI
MM 29.1	Wed	9:30-10:00	H24	Modelling and understanding the strength of grain boundaries based on ab-initio results — •REBECCA JANISCH
MM 46.1	Wed	18:00-18:30	H24	Brittle-ductile transitions - cracks and dislocations — •STEVE ROBERTS
MM 47.1	Wed	18:30-19:00	H24	Microscopic friction mechanisms on metal surfaces — \bullet ROLAND BENNEWITZ
MM 48.1	Thu	9:30–10:00	H24	Hydrogen embrittlement revisited by novel nano-mechanical approach — •AFROOZ BARNOUSH, MOHAMMAD ZAMANZADE, MASOUD ASGARI, ROY JOHNSEN, HORST VEHOFF
MM 57.1	Thu	15:00-15:30	H24	Micro- and macroplastic behavior of nanocrystalline Pd-Ag alloy in temperature range between 4 and $300K - \bullet$ Yulia Ivanisenko

Sessions

MM 1.1–1.1	Mon	9:30 - 10:00	H24	Invited Talk (Hauptvortrag): Dunin-Borkowski
MM 2.1–2.3	Mon	10:15 - 11:30	H4	Topical Session: TEM-Symposium - Joint Session with MI I
MM 3.1–3.5	Mon	10:15 - 11:30	H24	Computational Materials Modelling - Fundamentals
MM 4.1–4.3	Mon	10:15-11:30	H25	Topical Session: Quasicrystals & Complex Metallic Alloys I
MM $5.1 - 5.5$	Mon	10:15-11:30	H26	Functional Materials - Battery Materials I
MM 6.1–6.4	Mon	11:45 - 13:15	H4	Topical Session: TEM-Symposium - Joint Session with MI II
MM 7.1–7.5	Mon	11:45 - 13:00	H24	Computational Materials Modelling - Methods
MM 8.1–8.4	Mon	11:45 - 13:00	H25	Topical Session: Quasicrystals & Complex Metallic Alloys II
MM $9.1 - 9.5$	Mon	11:45 - 13:00	H26	Functional Materials - Battery Materials II
MM 10.1–10.1	Mon	15:00 - 15:30	H24	Invited Talk (Hauptvortrag): Schroers
MM 11.1–11.9	Mon	15:45 - 18:15	H4	Topical Session: TEM-Symposium - STEM

MM 12.1–12.10	Mon	15:45 - 18:15	H24	Computational Materials Modelling - Mechanical Properties
MM 13.1–13.9	Mon	15:45 - 18:00	H25	Topical Session: Quasicrystals & Complex Metallic Alloys III
MM 14.1–14.10	Mon	15:45 - 18:15	H26	Functional Materials - Hydrogen
MM 15.1–15.86	Mon	18:00 - 20:00	Poster E	Poster Session
MM 16.1–16.1	Tue	9:30 - 10:00	H24	Invited Talk (Hauptvortrag): Takeuchi
MM 17.1–17.4	Tue	10:15 - 11:30	H4	Topical Session: TEM-Symposium - HR Imaging & Analytic
				I
MM 18.1–18.5	Tue	10:15 - 11:30	H24	Computational Materials Modelling - Phase Stability I
MM 19.1–19.3	Tue	10:15 - 11:30	H25	Topical Session: Combinatorial Materials Science I
MM 20.1–20.5	Tue	10:15 - 11:30	H26	Transport & Diffusion I
MM 21.1-21.4	Tue	11:45 - 13:00	H4	Topical Session: TEM-Symposium - HR Imaging & Analytic
				II
MM 22.1–22.5	Tue	11:45-13:00	H24	Computational Materials Modelling - Phase Stability II
MM 23.1–23.4	Tue	11:45 - 13:00	H25	Topical Session: Combinatorial Materials Science II
MM 24.1–24.5	Tue	11:45 - 13:00	H26	Transport & Diffusion II
MM 25 1–25 3	Tue	15.00 - 16.00	H4	Topical Session: TEM-Symposium - Structure-Property
MM 26 1–26 4	Tue	15.00 - 16.00	H24	Computational Materials Modelling - Diffusion & Kinetics I
MM 27 1–27 2	Tue	15.00 - 16.00	H25	Topical Session: Combinatorial Materials Science III
MM 28 1–28 4	Tue	15.00 - 16.00	H26	Transport & Diffusion III
MM 29 1–29 1	Wed	9:30-10:00	H24	Invited Talk (Hauptvortrag): Janisch
MM 30 1-30 5	Wed	10.15 - 11.30	H4	Topical Session: Fundamentals of Fracture - Modelling Inter-
WIW 50.1 50.5	weu	10.10 11.00	114	aranular Fracture
MM 31 1_31 5	Wed	10.15-11.30	H94	Computational Materials Modelling - Diffusion & Kinetics II
MM 22 1 22 4	Wed	10.15 - 11.30 10.15 - 11.20	1124 H95	Topical Session: TEM Symposium Structure Droperty / In
WIWI 52.1-52.4	weu	10.15-11.50	1125	Situ I
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$MM \ 33.1 - 33.5$	Wed	10.15 - 11.50 11.45 - 12.00	1120 H4	Topical Sossion, Fundamentals of Fracture Fracture at the
WIM 54.1-54.5	weu	11.45-15.00	114	Atomistia Saslo
MM 25 1 25 5	Wed	11.45 12.00	<u>цо</u> 4	Computational Materiala Modelling Dhonong & Dhogo Sta
MM 55.1-55.5	wea	11:40-10:00	1124	biliter
MM 26 1 26 4	Wed	11.45 12.00	HOF	Dility Tenical Section: TEM Summarium Statistica Deponents / In
MM 30.1-30.4	wea	11:45-15:00	H20	10pical Session: 1 EM-Symposium - Structure-Property / In-
MM 97 1 97 5	Wed	11.45 12.00	1196	Situ II Mashaniaal Duan antias I
MM 37.1 - 37.3	wea	11:45-13:00	H20	Tranical Properties I
MM 38.1-38.4	wea	19:00-10:19	П4	10pical Session: Fundamentals of Fracture - Atomistic Mod-
MM 20 1 20 5	Wed	15.00 16.15	1194	elling Computational Materials Madelling Transport Evoltations
MM 59.1-59.5	wea	10:00-10:10	Π24	Computational Materials Modelling - Transport, Excitations,
MM 40 1 40 4	11 71	15.00 16.15	1105	Time Dependence I Transie Services TEM Service estimates In Sites I
MM 40.1-40.4	wea	15:00-16:15	H25	Topical Session: TEM-Symposium - In-Situ I
MM 41.1-41.5	wea	15:00-16:15	H26	mechanical Properties II
MM 42.1–42.4	Wed	16:30-17:45	H4	Topical Session: Fundamentals of Fracture - Continuous Mod-
	TT 7 1	10.00 15 45	TIO (
MM 43.1–43.5	Wed	16:30-17:45	H24	Computational Materials Modelling - Transport, Excitations,
			TTOF	Time Dependence II
MM 44.1–44.4	Wed	16:30-17:45	H25	Topical Session: TEM-Symposium - In-Situ II
MM 45.1-45.5	Wed	16:30-17:45	H26	Nanomaterials - Nanospheres & Fibres
MM 46.1–46.1	Wed	18:00-18:30	H24	Invited Talk (Hauptvortrag): Roberts
MM 47.1–47.1	Wed	18:30-19:00	H24	Invited Talk (Hauptvortrag): Bennewitz
MM 48.1–48.1	Thu	9:30-10:00	H24	Invited Talk (Hauptvortrag): Barnoush
MM 49.1–49.4	Thu	10:15-11:30	H4	Topical Session: Fundamentals of Fracture - Novel Experi-
	_			mental Techniques I
MM 50.1–50.5	Thu	10:15-11:30	H24	Computational Materials Modelling - Defects & Interfaces I
MM 51.1–51.5	Thu	10:15-11:30	H25	Nanomaterials - Nanocrystalline & Porous Materials I
MM 52.1–52.5	Thu	10:15-11:30	H26	Phase Transformations I
MM 53.1–53.5	Thu	11:45 - 13:00	H4	Topical Session: Fundamentals of Fracture - Novel Experi-
				mental Techniques II
MM 54.1–54.5	Thu	11:45 - 13:00	H24	Computational Materials Modelling - Defects & Interfaces II
MM $55.1-55.5$	Thu	11:45 - 13:00	H25	Nanomaterials - Nanocrystalline & Porous Materials II
MM 56.1–56.5	Thu	11:45 - 13:00	H26	Phase Transformations II
MM 57.1–57.1	Thu	15:00 - 15:30	H24	Invited Talk (Hauptvortrag): Ivanisenko
MM $58.1 - 58.4$	Thu	15:45 - 17:00	H4	Topical Session: Fundamentals of Fracture - Fatigue Fracture
MM $59.1 - 59.5$	Thu	15:45 - 17:00	H24	Computational Materials Modelling - Phase Stability III

MM 60.1–60.5	Thu	$\begin{array}{c} 15{:}45{-}17{:}00\\ 15{:}45{-}17{:}00\\ 17{:}15{-}18{:}45\end{array}$	H25	Nanomaterials - Nanoparticles
MM 61.1–61.5	Thu		H26	Liquid & Amorphous Metals I
MM 62.1–62.5	Thu		H4	Topical Session: Fundamentals of Fracture - Stochastic As-
MM 63.1–63.7 MM 64.1–64.6 MM 65.1–65.7	Thu Thu Thu	$\begin{array}{c} 17{:}15{-}19{:}00\\ 17{:}15{-}18{:}45\\ 17{:}15{-}19{:}00\end{array}$	H24 H25 H26	pects Computational Materials Modelling - Phase Stability IV Nanomaterials - Miscellaneous Liquid & Amorphous Metals II

Topical session "Fundamentals of Fracture"

Organizers: Prof. Dr. Erik Bitzek (Universität Erlangen-Nürnberg), Prof. Dr. Sandra Korte (Universität Erlangen-Nürnberg), Prof. Dr. Peter Gumbsch (Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg)

This symposium is intended as an international forum for the presentation and discussion of the latest scientific developments related to fundamental mechanisms and physics of fracture. The general theme of the Fundamentals of Fracture Symposium is to cover all aspects of fracture at a fundamental level, rather than specific engineering approaches. We aim at bringing together specialists from the fields of solid state physics, materials science, continuum mechanics, statistical physics and mathematics.

The symposium will cover theory, multi-scale modelling and recent experimental advances related to interaction of cracks with the microstructure, interplay of fracture and plasticity, initiation of fracture, fracture of nanostructures and -materials, influence of constraints on fracture, fracture of disordered materials, Statistical aspects of fracture, dynamic fracture, environmental effects on fracture.

Topical session "TEM-Symposium: Using Transmission Electron Microscopy to Unravel the Mysteries of Materials"

Organizers: Prof. Cynthia A. Volkert (Universität Göttingen), Prof. Dr. Joachim Mayer (RWTH Aachen)

Recent advances in transmission electron microscopy have led to significant improvements in spatial and energy resolution, and have also prompted the development of new tools and techniques. The result has been a significant step forward in our ability to interrogate atomic and electron structure at the Angstrom level. Particularly the rapid development of in-situ methods has allowed the observation of dynamic processes and the direct correlations between structure and properties. The goal of the symposium is to bring together and stimulate discussion among researchers from various disciplines (physics, chemistry, materials science, mineralogy) who develop and apply advanced TEM techniques to studying and understanding materials.

A Joint session with division "Microprobes", MI, takes place on Monday morning from 10:15 to 13:15 in H4 within this Topical session.

Topical session "Combinatorial Materials Science"

Organizers: Prof. Dr. Jörg Neugebauer (MPIE Düsseldorf), Prof. Dr. Ralf Drautz (Ruhr Universität Bochum), Prof. Dr. Jochen Schneider (RWTH Aachen)

In this symposium we address the discovery and optimization of materials through high-throughput experimentation. Suggested topics for contributions are: combinatorial synthesis of thin film and bulk materials libraries, high-throughput characterization of materials, up-scaling from combinatorial data to novel materials.

Topical session "Quasicrystals and Complex Metallic Alloys"

Organizer: Prof. Dr. Hans-Rainer Trebin (Universität Stuttgart)

Invited talks of the joint symposium SYTS (DF, DS, HL, MA, MI, MM, TT) "Thermoelectric and Spincaloric Transport in Nanostructures"

See SYTS for the full program of the symposium.

SYTS 1.1	Wed	9:30 - 10:00	H1	Transport in Old and New Thermoelectric Materials — •DAVID SINGH
SYTS 1.2	Wed	10:00-10:30	H1	Binary oxide structures as model systems for thermoelectric transport
				— •Peter J. Klar, Christian Heiliger
SYTS 1.3	Wed	10:30-11:00	H1	Functional oxides films: from single crystals to polycrystalline sub-
				strates — • Wilfrid Prellier
SYTS 1.4	Wed	11:00-11:30	H1	The Planar Nernst Effect and the Search for Thermal Spin Currents in
				Ferromagnetic Metals — •BARRY ZINK
SYTS 1.5	Wed	11:30-12:00	H1	Tunneling magneto thermopower in magnetic tunnel junction nanopil-
				lars — Niklas Liebing, Santiago Serrano-Guisan, Patryk Krzysteczko,
				KARSTEN ROTT, GÜNTER REISS, JÜRGEN LANGER, BERTHOLD OCKER, •HANS
				Werner Schumacher

Invited talks of the joint symposium SYMM (BP, CPP, DY, MM) "Computational Challenges in Scale-Bridging Modeling of Materials"

See SYMM for the full program of the symposium.

Thu	9:30-10:00	H1	Challenges for first-principles based computation of properties of oxide materials — \bullet KARSTEN ALBE
Thu	10:00-10:30	H1	Deformation and Fracture of Solids: Tough Nuts at Atomic and Contin-
			uum Scales — •Peter Gumbsch, Matous Mrovec, Kinshuk Srivastava,
			Daniel Weygand
Thu	10:30 - 11:00	H1	Crucial Issues and Future Directions of Through-Process Modeling —
			•Guenter Gottstein
Thu	11:00-11:30	H1	Adaptive Resolution Simulations for Soft Matter: Applications and
			New Developments — •Kurt Kremer
Thu	11:30-12:00	H1	Materials by design — • MARKUS BUEHLER
	Thu Thu Thu Thu Thu Thu	Thu 9:30–10:00 Thu 10:00–10:30 Thu 10:30–11:00 Thu 11:00–11:30 Thu 11:30–12:00	Thu 9:30-10:00 H1 Thu 10:00-10:30 H1 Thu 10:30-11:00 H1 Thu 11:00-11:30 H1 Thu 11:30-12:00 H1

Invited talks of the joint symposium SYES (O, DS, HL, MA, MM, TT) "Frontiers of Electronic Structure Theory: Discovery of Novel Functional Materials"

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30 - 10:00	H1	Molecular dynamics simulation of nucleation and growth of crystals from
				$solution - \bullet Michele Parrinello$
SYES 1.2	Fri	10:00-10:30	H1	Describing, understanding, and discovering hybrid materials from first
				principles — •Claudia Draxl
SYES 1.3	Fri	10:30-11:00	H1	Mapping the Electronic Structure Landscape for Materials Discovery —
				•Krishna Rajan
SYES 1.4	Fri	11:00-11:30	H1	New ferroelectrics and antiferroelectrics by design — •KARIN RABE
SYES 1.5	Fri	11:30-12:00	H1	The Materials Project: The design of materials using high-throughput
				ab initio computations — •GERBRAND CEDER

Annual General Meeting of the Metal and Material Physics Division

Wednesday 19:30–20:30 H24

This year's general meeting of the Metal and Materials Physics Division (FV MM) is taking place on Wednesday at 19:30 in room H24 after the invited talks (Hauptvorträge) by S. Roberts and R. Bennewitz and the following social gathering. The meeting will be opened with a short welcome address and the report of the chairman of the Metal and Materials Physics Division (AGMM). Afterwards, all attendees are invited to elect a new Chairman of the "Fachverband Metall- und Materialphysik" and to suggest symposia and speakers which could be invited for the next spring meeting in Dresden, 30th March to 04th April 2014. Everybody is highly welcome to join the social gathering and participate at the annual meeting directly afterwards.