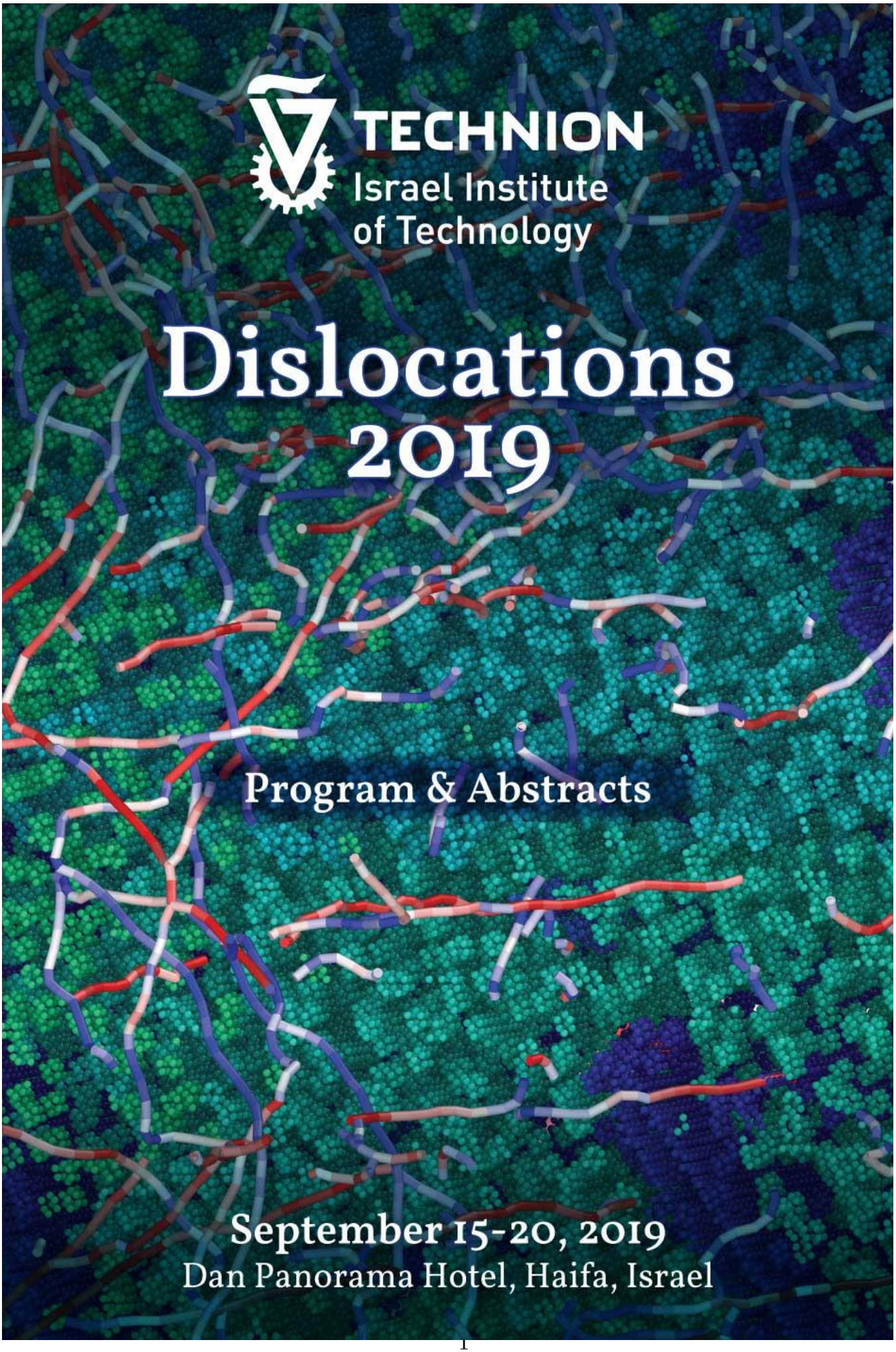
TECHNION
Israel Institute
of Technology
Dislocations
2019
Program & Abstracts
September 15-20, 2019
Dan Panorama Hotel, Haifa, Israel

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WELCOME

Dear Colleagues,

On behalf of the organizing committee, we warmly welcome you to the 6th edition of the Dislocations conference series, held during 15-20 September, 2019, at the Dan Panorama hotel, Haifa, Israel.

The conference series started on June 2000 at the National Institute of Standards and Technology (MD, USA). Since then, "Dislocations" conferences were held at La Colle sur Loup (France) in 2004, Hong Kong in 2008, Budapest (Hungary) in 2012 and at West Lafayette (USA) on 2016.

We have put together an exciting program combining the contributions of world-renowned scholars with the talks of young researchers, presenting experimental observations, computer simulations and theoretical models of dislocations and plasticity. The diverse list of authors, and especially the contribution of young scientists, is the best proof that this is still a growing field, with many stimulating questions for Dislocations conferences in the future. In the spirit of previous conferences, we have kept the traditional Dislocations format of a single session conference. On behalf of the organizing committee, I would like to thank all speakers, poster presenters, the International Advisory board and our sponsors, who are contributing to the success of this conference.

During your stay, we hope that you will benefit from a stimulating scientific meeting but also take this opportunity to visit some of the interesting and unique sites in Haifa and in Israel. Haifa, the port city in Northern Israel is the third largest city and one of the prettiest, built on the slopes of Mount Carmel overlooking the Mediterranean Sea. It is a unique multicultural city in which people of various faiths live peacefully and work together.

Thank you for joining us at Dislocations 2019 in Haifa.

Dan Mordehai,
Dislocations 2019 – Chairman
Technion – Israel Institute of Science

COMMITTEES

Local Organizing Committee

Dan Mordehai, Technion – Israel Institute of Technology *(Conference Chairman)*
Eugen Rabkin, Technion – Israel Institute of Technology
Roni Shneck, Ben-Gurion University of the Negev

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Erik Bitzek, Friedrich-Alexander University Erlangen-Nuremberg, Germany
Marc Legros, CEMES-CNRS Toulouse, France
Yoji Shibutani, Osaka University, Japan

TIMETABLE

Sunday, September 15, 2019		
17:30-20:00	Registration and distribution of material	Foyer
19:00-21:00	***Welcome Reception***	Pythagoras Hall
Monday, September 16, 2019		
08:45-09:15	OPENING SESSION	Alon Hall
09:15-10:30	**Session 1 – Dislocation-solutes interaction (1)**	Alon Hall
10:30-11:00	Coffee Break	
11:00-12:45	**Session 2 – Dislocation-solutes interaction (2) & Dislocation Properties (1a)**	Alon Hall
12:45-14:15	Lunch Break	Dining Room
14:15-16:00	**Session 3 - Dislocation Properties (1b)**	Alon Hall
16:00-16:30	Coffee Break	Foyer
16:30-18:15	**Session 4 - Dislocation Properties (2)**	Alon Hall
Tuesday, September 17, 2019		
09:00-10:30	**Session 5 – Work hardening**	Alon Hall
10:30-11:00	Coffee Break	Foyer
11:00-12:15	**Session 6 – Dislocation Dynamics & Dislocation Climb**	Alon Hall
12:15-14:00	Lunch Break	Dining Room
14:00-15:30	**Session 7 – Dislocation Dynamics, Irradiation & Hydrogen Embrittlement**	Alon Hall
15:30-16:15	Coffee Break	Foyer
16:15-17:00	**Session 8 – Nanoindentation**	Alon Hall
17:00-18:00	**Poster Flash Presentations**	Alon Hall
20:00-22:00	**Poster Viewing Session** (wine & beer)	Pythagoras Hall
Wednesday, September 18, 2019		
09:00-10:30	**Session 9 – Continuum Models of Dislocations**	Alon Hall
10:30-11:00	Coffee Break	Foyer
11:00-12:30	**Session 10 – Continuum Models of Dislocations & Data Science**	Alon Hall
12:30-13:45	Lunch Break	Dining Room
13:45-19:00	***Conference Tour to Akko (Acre)*** *Departure: From the Dan Panorama hotel*	
Thursday, September 19, 2019		
09:00-10:30	**Session 11 – Grain and twin boundaries (1)**	Alon Hall
10:30-11:00	Coffee Break	Foyer
11:00-12:15	**Session 12 – Grain and twin boundaries (2)**	Alon Hall
12:15-13:45	Lunch Break	Dining Room
13:45-15:15	**Session 13 – Grain and twin boundaries (3) & Brittle-to-Ductile Transition**	Alon Hall
15:15-15:45	Coffee Break	Foyer
15:45-16:45	**Session 14 – Dislocations in Alloys**	Alon Hall
16:45-18:15	Free Time	
19:00-20:00	**Keynote Lecture: Dan Shechtman** Nobel Prize Laureate in Chemistry 2011 *Departure: 18:15 from the Dan Panorama hotel*	Technion Dan-Kahn Bldg. Hall 16)
20:00-22:00	***Conference Dinner*** (at the Technion)	
Friday, September 20, 2019		
09:00-10:45	**Session 15 – Dislocations in Nanostructures (1)**	Alon Hall
10:45-11:15	Coffee Break	Foyer
11:15-12:30	**Session 16 – Dislocations in Nanostructures (2)**	Alon Hall
12:00-12:15	**Closing Remarks**	Alon Hall
12:15	Light Lunch	

GENERAL INFORMATION

Conference Venue
Dan Panorama Hotel
107 Ha'Nassi Blvd.
Haifa, Israel
Tel: +972(0)4-835-2222

Internet
Wi-Fi internet connection is available at the Dan Panorama hotel free of charge in all public areas and hotel rooms.
Network: dph

Language
The official language of the conference is English.

Registration and Hospitality Desk
Diesenhaus-Unitours will operate the registration & hospitality desk at the
Dan Panorama Hotel throughout the conference, at the following times:
Sunday: 17:30-20:00
Monday-Friday: from 08:30 during session hours.

Badges & Tickets
Please wear your name badge at all conference sessions and events and present the tickets at the entrance to the Welcome Reception and Conference Dinner.

Conference Abstracts
The on-line program with link to abstracts as well as a PDF file of the program and abstracts are available on the conference website, program page https://dislocations2019.net.technion.ac.il/program/

Speakers and Session Chairpersons
Session chairpersons and speakers are requested to meet with each other 10 minutes prior to the commencement of their respective sessions, in the session hall. Speakers should not depart from the time allocated for their presentation and allow time for some questions.

Data Projection
Please bring your presentation on a USB Memory stick (using the USB port in the computer) and give it to the A/V technician in the session hall, at least one hour before the start of your session. The A/V technician will load your presentation onto the conference computer. If using your own laptop, please coordinate it in advance with the A/V technician.

Instructions for Poster Presenters
Set-up: Tuesday - from 12:30, during lunch break (Pythagoras Hall)
Removal: Tuesday, after end of poster session (~22:00)
Please mount your poster on the board number listed in this program booklet.

Conference Documents at Airport
We recommend that you keep the Conference documents handy, in order to expedite the security process during check-in for your departure flight. It is recommended to arrive at Ben-Gurion Airport 3 hours prior to departure.

CONFERENCE TOUR TO AKKO (Acre)

Wednesday, September 18, 2019
Departure: 13:45 from the lobby of the Dan Panorama hotel.
Drop-off - two options: At the German Colony in Haifa, where you can have dinner (own expense), or proceed with the bus to the conference hotels. *Comfortable walking shoes, sunglasses, hat, suntan lotion, are recommended.*

Start the tour with a view from the upper terrace of the **Bahái Gardens**, a Haifa landmark and one of the most visited sites in the Middle East. The magnificent Gardens comprise a staircase of nineteen terraces extending all the way up the northern slope of Mount Carmel. At its heart stands the golden-domed Shrine of the Báb, which is the resting place of the Prophet-Herald of the Bahá'í Faith.

Continue to **Akko (Acre)**, located north of Haifa on the Mediterranean coast. Akko is a city that has been shaped by the Romans, Ottomans, Crusaders, Mamelukes, Byzantines, and British, and fittingly is today home to a brilliantly coexistent mixed population of Jews, Christians and Muslims and is also home to part of the Bahai World Center (the other part being in Haifa).

The Old City of Akko is a UNESCO World Heritage Site in recognition of the remains of the Crusader town and because it is one of a very few Ottoman walled towns with citadels, mosques, khans and baths, which have been preserved. In Akko, these sites were built on top of the ruins of the Crusader structures. Alexander the Great, Julius Caesar, and Marco Polo are mentioned as some of the giants in history that visited this ancient sea-port city. Napoleon Bonaparte tried to conquer it, but retreated after two months of siege and failed attempts to storm the city's walls. The city today is a meeting place for East and West, new and old, beauty and ruins, and offers a variety of sites, such as the colorful market ("shuk"), authentic restaurants, boat rides and a variety of cultural events, which make Akko a bustling city and a unique place to visit.

PROGRAM

SUNDAY, SEPTEMBER 15, 2019

17:30-20:00 Registration and distribution of material *Foyer*

19:00-21:00 Welcome Reception ***Pythagoras Hall***

MONDAY, SEPTEMBER 16, 2019

08:45-09:15 OPENING SESSION — Alon Hall

Welcome:

Dan Mordehai, *Dislocations 2019 Conference Chair*

Representative of the Israel Ministry of Science & Technology

09:15-10:30 Session 1 – Dislocation-solute interaction (1) — Alon Hall

Chair: **David Rodney,** University of Lyon, Lyon, France

09:15 *Invited Lecture*
Dislocations and strengthening in random BCC alloys

William Curtin, F. Maresca
Mechanical Engineering, EPFL, Lausanne, Switzerland

09:45 *Invited Lecture*
Simulating dislocation-solute co-evolution in body-centered cubic metals on diffusive timescales

Yue Zhao[1], Lucile Dezerald[2], **Jaime Marian**[1]
[1]*Materials Science and Engineering, UCLA, Los Angeles, CA, USA*
[2]*Institut Jean Lamour, Université de Lorraine, Nancy, France*

10:15 **Large-scale molecular dynamics simulations reveal length-dependent dislocation mobilities in Fe-Cr-Ni austenitic stainless steel**

Ryan Sills[1], Michael Foster[2], Xiaowang Zhou[2]
[1]*Gas Transfer Systems, Sandia National Laboratories, Livermore, CA, USA*
[2]*Mechanics of Materials, Sandia National Laboratories, Livermore, CA, USA*

10:30-11:00 Coffee Break

11:00-12:45 Session 2 – Dislocation-solute interaction (2) & Dislocation Properties (1a) — *Alon Hall*

Chair: **Jaime Marian,** University of California Los Angeles, Los Angeles, CA, USA

11:00 *Invited Lecture*
Multiscale modelling of precipitation hardening in metallic alloys

Javier LLorca
IMDEA Materials Institute & Polytechnic University of Madrid, Madrid, Spain

11:30 **Plasticity and dislocation mechanisms in aluminium alloys containing precipitate free zones**

Inga Ringdalen[1], Sigurd Wenner[1], Jesper Friis[1], Emil Christiansen[2,3], Jonas Frafjord[2,3], Mikhail Khadyko[4], Odd Sture Hopperstad[2,4], Randi Holmestad[2,3]
[1]*Department of Materials and Nanotechnology, Sintef Industry, Trondheim, Norway*
[2]*Centre for Advanced Structural Analysis (CASA), Norwegian University of Science and Technology, Trondheim, Norway*
[3]*Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway*
[4]*Department of Structural Engineering, Norwegian University of Science and Technology, Trondheim, Norway*

11:45 **Atomistic phase field chemomechanical modeling of defect-solute interaction in metallic alloys**

Bob Svendsen[1,3], Jaber Rezaei Mianroodi[1,3], Pratheek Shanthraj[2]
[1]*Material Mechanics, RWTH Aachen University, Aachen, Germany*
[2]*School of Materials, University of Manchester, Manchester, UK*
[3]*Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany*

12:00 **The effect of multiple species in solute strengthening in aluminium – A molecular dynamics study**

Jonas Frafjord[1,4], Jesper Friis[2,4], Randi Holmestad[1,4], Bjørn Holmedal[3], Inga Ringdalen[2,4]
[1]*Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway*
[2]*Industry, SINTEF, Trondheim, Norway*
[3]*Department of Materials Science and Engineering, Norwegian University of Science and Technology, Trondheim, Norway*
[4]*NA, SFI Center for Advanced Structural Analysis, Trondheim, Norway*

12:15 *Invited Lecture*
Mobility of screw dislocations in hexagonal close-packed zirconium and titanium

Emmanuel Clouet[1], Nermine Chaari[1], David Rodney[2], Daniel Caillard[3]
[1]*SRMP, CEA Saclay, Gif-syr-Yvette, France*
[2]*ILM, Université Lyon 1 / CNRS, Lyon, France*
[3]*CEMES, CNRS, Toulouse, France*

12:45-14:15 Lunch Break — ***Dining Room***

14:15-16:00 Session 3 - Dislocation Properties (1b) — Alon Hall

Chair: **Vasily Bulatov,** Lawrence Livermore National Laboratory, Livermore, CA, USA

14:15 *Invited Lecture*
Non-Schmid effects in BCC metals from first principles

Lucile Dezerald[1,2], Antoine Kraych[3], Bassem Ben Yahia[1,2], Emmanuel Clouet[4], Lisa Ventelon[4], François Willaime[5], David Rodney[3]
[1]*Institut Jean Lamour, Université de Lorraine, Nancy, France*
[2]*LabEx DAMAS, Université de Lorraine, Metz, France*
[3]*Institut Lumière Matière, Université Lyon 1, Villeurbanne, France*
[4]*DEN-Service de Recherches de Métallurgie Physique, CEA Saclay, Gif-Sur-Yvette, France*
[5]*DEN-Département des Matériaux pour le Nucléaire, CEA Saclay, Gif-Sur-Yvette, France*

14:45 **Origin of anomalous slip in bcc metals**

Roman Gröger[1], Vaclav Vitek[2]
[1]*Institute of Physics of Materials and CEITEC IPM, Czech Academy of Sciences, Brno, Czech Republic*
[2]*Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA, USA*

15:00 **Effect of solutes on the core structure and mobility of dislocations in bcc metals**

Lisa Ventelon[1], Berengere Luthi[1], **François Willaime**[3], David Rodney[2]
[1]*Service de Recherches de Métallurgie Physique, CEA, Gif-sur-Yvette, France*
[2]*Institut Lumière Matière, CNRS-Université Claude Bernard, Lyon, France*
[3]*Department of Materials for Nuclear Energy, CEA, Gif-sur-Yvette, France*

15:15 **Core structure and mobility of mixed ½ [111] dislocations in bcc metals**

Tapaswani Pradhan[1], Anastasiia Kholtobina[2], **Lorenz Romaner**[2], Matous Mrovec[1], Ralf Drautz[1]
[1]*Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, Bochum, Germany*
[2]*Department of Materials Simulation, Materials Center Leoben Forschung GmbH, Leoben, Austria*

15:30 **Atomistic simulations of dislocations in iron-chromium alloys**

Matous Mrovec, Sergei Starikov, Ralf Drautz
ICAMS, Ruhr-Universität Bochum, Bochum, Germany

15:45 **Plastic deformation of chromium single crystals at 77 K**

Jakub Holzer[1], Roman Gröger[1], Zdeněk Chlup[2]
[1]*Department of Multiscale Modelling and Measurements of Physical Properties, Institute of Physics of Materials and CEITEC IPM, Academy of Sciences of the Czech Republic, Brno, Czech Republic*
[2]*Department of Brittle Fracture, Institute of Physics of Materials of Czech Academy of Sciences, Brno, Czech Republic*

16:00-16:30 Coffee Break

16:30-18:15 Session 4 - Dislocation Properties (2) — Alon Hall

Chair: **Wei Cai,** Stanford University, Stanford, CA, USA

16:30 *Invited Lecture*
Linear complexion formation driven by local stress concentrations near dislocations

Timothy Rupert
Materials Science and Engineering, University of California, Irvine, Irvine, CA, USA

17:00 *Invited Lecture*
Thermal fluctuations of dislocations

Pierre-Antoine Geslin[1], David Rodney[2]
[1]*Mateis, INSA Lyon, Lyon, France*
[2]*Institut Lumière Matière, Université Lyon 1, Lyon, France*

17:30 **Fundamental reactions between prismatic loops in stochastic dislocation dynamics**

Max Boleininger[2], Yang Li[1], Christian Robertson[1], Laurent Dupuy[1], Sergei L. Dudarev[2]
[1]*DEN-Service de Recherches Métallurgiques Appliquées, CEA, Paris-Saclay, France*
[2]*Culham Centre for Fusion Energy, UK Atomic Energy Authority, Abingdon, UK*

17:45 **A molecular-dynamics investigation of single dislocations**

Eyal Oren[1], Eyal Yahel[2], Guy Makov[1]
[1]*Department of Materials Engineering, Ben-Gurion University of the Negev, Beer-Sheva, Israel*
[2]*Physics Department, NRCN, Beer-Sheva, Israel*

18:00 **Atomistic simulation of jog pair in magnesium oxide**

Jian-Hui Zhai, Pierre Hirel, Philippe Carrez
Department of Physics, Universite de Lille, UMR CNRS 8207 Umet, Lille, France

TUESDAY, SEPTEMBER 17, 2019

09:00-11:00 Session 5 – Work Hardening — Alon Hall

Chair: **Giacomo Po,** University of Miami, Coral Gables, FL, USA

09:00 *Invited Lecture*

Three stages of work hardening in full atomistic details. Seriously

Luis Zepeda-Ruiz[1], Alexander Stukowski[2], Tomas Oppelstrup[1], Nathan Barton[3], Rodrigo Freitas[1,4,5], Nicolas Bertin[1], **Vasily Bulatov**[1]
[1]*Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, Livermore, CA, USA*
[2]*FG Materialmodellierung, Technische Universität Darmstadt, Darmstadt, Germany*
[3]*Engineering Directorate, Lawrence Livermore National Laboratory, Livermore, CA, USA*
[4]*Materials Science and Engineering, University of California Berkeley, Berkeley, CA, USA*
[5]*Materials Science and Engineering, Stanford University, Stanford, CA, USA*

09:30 Plastic relaxation in tantalum single crystals strained far from equilibrium

Luis Zepeda-Ruiz, Vasily Bulatov
Materials Science Division, Lawrence Livermore National Laboratory, Livermore, CA, USA

09:45 The molecular dynamics study of the mechanisms and kinetics of plasticity in aluminum and copper alloys under high-strain rate

Ilya Bryukhanov
Institute of Mechanics, Lomonosov Moscow State University, Moscow, Russia

10:00 *Invited Lecture*

Microstructural origin of work hardening in FCC Cu single crystals

Wei Cai[1], Shamseddin Akhondzadeh[1], Ryan Sills[2], Nicolas Bertin[1], Minju Kang[3], Vignesh Kannan[3], K. T. Ramesh[3]
[1]*Mechanical Engineering, Stanford University, Stanford, CA, USA*
[2]*Gas Transfer Systems, Sandia National Laboratories, Livermore, CA, USA*
[3]*Hopkins Extreme Materials Institute, Johns Hopkins University, Baltimore, MD, USA*

10:30-11:00 Coffee Break

TUESDAY, SEPTEMBER 17, 2019

11:00-12:15 Session 6 – Dislocation Dynamics and Dislocation Climb — Alon Hall

Chair: **Katrin Schulz,** Karlsruhe Institute of Technology, Karlsruhe, Germany

11:00 **Dislocation patterns and the similitude principle: A 3D-DD simulations investigation**

Benoit Devincre, Francesca Boioli, Riccardo Gatti
LEM, CNRS-ONERA, CNRS, Chatillon, France

11:15 **Grain size effects on back stresses induced by GND: A Dislocations Dynamics study**

Ghiath Monnet[2], Maoyuan Jiang[2], Benoit Devincre[1]
[1]*LEM, CNRS - ONERA, Chatillon, France*
[2]*MMC, EDF R&D, Moret, France*

11:30 *Invited Lecture*
Dislocation climb and annealing in 3D dislocation dynamics simulations

Po Giacomo[1,2], Yue Huang[2], Nasr Ghoniem[2]
[1]*Mechanical and Aerospace Engineering, University of Miami, Miami, FL, USA*
[2]*Mechanical and Aerospace Engineering, University of California Los Angeles, Los Angeles, CA, USA*

12:00 **A new method to investigate dislocation self-climb dominated by core diffusion**

Fengxian Liu[1], Edmund Tarleton[1], A.C.F. Cocks[2]
[1]*Department of Materials, University of Oxford, Oxford, UK*
[2]*Department of Engineering Science, University of Oxford, Oxford, UK*

12:15-14:00 Lunch Break — ***Dining Room***

14:00-15:30 Session 7 – Dislocation Dynamics, Irradiation & Hydrogen Embrittlement — Alon Hall

Chair: **Emmanuel Clouet,** CEA Saclay, Gif-sur-Yvette, France

14:00 *Invited Lecture*
Advances in dislocation microstructure prediction: a FFT-based Dislocation Dynamics approach

Riccardo Gatti[1], Francesca Boioli[1], Benoit Devincre[1], Lionel Gélébart[2], Laurent Dupuy[2]
[1]*LEM UMR 104, CNRS-ONERA, Châtillon, France*
[2]*SRMA, CEA, Saclay, France*

14:30 **Modelling the plasticity of zirconium hydrides**

Luca Reali[1], Daniel S. Balint[2], Mark R. Wenman[3], Adrian P. Sutton[1]
[1]*Department of Physics, Imperial College London, London, UK*
[2]*Department of Mechanical Engineering, Imperial College London, London, UK*
[3]*Department of Materials, Imperial College London, London, UK*

14:45 **Hydrogen embrittlement defactant concept applied to discrete dislocation dynamics**

Jan Inge Meling, Afrooz Barnoush
Department of Mechanical and Industrial Engineering, Norwegian University of Science and Technology, Trondheim, Trøndelag, Norway

15:00 **Multi-scale approach of the consequences of hydrogen on cyclic behaviour of nickel single crystal**

Guillaume Hachet[1,3], Abdelali Oudriss[1], Afrooz Barnoush[2], Rémy Milet[1], Di Wan[2], Arnaud Metsue[1], Xavier Feaugas[1]
[1]*LaSIE UMR CNRS 7356, Université de La Rochelle, La Rochelle, France*
[2]*Department of Mechanical and Industrial Engineering, Norwegian University of Science and Technology, Trondheim, Norway*
[3]*CEA - Saclay, Service de Recherches de Métallurgie Physique, Gif-sur-Yvette, France*

15:15 **Deformation mechanisms and twin formation observed in Irradiated ferritic/martensitic steels**

Yong Dai[1], Kun Wang[1], Min Xia[2], Liang Wang[3]
[1]*Laboratory for Nuclear Materials, Paul Scherrer Institut, Villigen, Switzerland*
[2]*Institute of Nuclear Materials, University of Science & Technology Beijing, Beijing, China*
[3]*College of Science, Hunan Agricultural University, Changsha, China*

15:30-16:15 Coffee Break

16:15-17:00 Session 8 – Nanoindentation — Alon Hall

Chair: **Timothy Rupert,** University of California, Irvine, CA, USA

16:15 *Invited lecture*

Dislocation structure and grain boundary motion induced by nanindentations on STO and W

Karsten Durst, Farhan Javaid
Materials Science, Technische Universität Darmstadt, Darmstadt, Germany

16:45 **Plasticity in Au crystals studied by In-situ nano-indentation coupled with bragg coherent diffraction imaging**

Stephane Labat[1], Florian Lauraux[1], Thomas Cornelius[1], Marie-Ingrid Richard[1], Oleg Kovalenko[2], Eugen Rabkin[2], Olivier Thomas[1]
[1]*Physics Department, IM2NP - CNRS 7334, Aix Marseille University, Marseille, France*
[2]*Materials Science and Engineering, Technion – Israel Institute of Technology, Haifa, Israel*

17:00-18:00 Poster Flash Presentations — Alon Hall

20:00-22:00 Poster Viewing Session (wine & beer) — Pythagoras Hall

See list of posters on page 25

WEDNESDAY, SEPTEMBER 18, 2019

09:00-10:30 Session 9 – Continuum Models of Dislocations — Alon Hall

Chair: **Stefan Sandfeld,** TU Freiberg, Freiberg, Germany

09:00 *Invited Lecture*
Dislocation patterning in finite deformation dislocation mechanics and towards plasticity without phenomenological assumptions

Rajat Arora[1], Sabyasachi Chatterjee[1], Giacomo Po[2], Xiaohan Zhang[1], **Amit Acharya**[1], Nasr Ghoniem[2]
[1]*Civil and Environmental Engineering, Carnegie Mellon University, Pittsburgh, PA, USA*
[2]*Mechanical and Aerospace Engineering, University of California, Los Angeles, CA, USA*

09:30 *Invited Lecture*
A Phase Field approach to describe the collective properties of dislocations

Istvan Groma
Department of Materials Physics, Eotvos University Budapest, Budapest, Hungary

10:00 **Large deformation continuum dislocation theory: kinks, jogs and dislocation--vacancy interaction**

Thomas Hochrainer, Benedikt Weger
Institute of Strength of Materials, TU Graz, Graz, Austria

10:15 **Strain gradient influence on dislocation dynamics**

Paulo Pereira, Sérgio Apolinário
Departamento de Física, Universidade Federal de Pernambuco, Recife, Brazil

10:30-11:00 Coffee Break

11:00-12:30 Session 10 – Continuum Models of Dislocations & Data Science Alon Hall

Chair: **Seunghwa Ryu,** Korea Advanced Institute of Science and Technology, Daejeon, South Korea

11:00 *Invited Lecture*
Dislocation network evolution in continuum dislocation dynamics

Katrin Schulz[1], Markus Sudmanns[1], Kolja Zoller[1], Peter Gumbsch[1,2]
[1]*Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany*
[2]*Fraunhofer Institute for Mechanics of Materials, (IWM), Freiburg, Germany*

11:30 *Invited Lecture*
From experiment to simulation and back – data science approaches for understanding plasticity

Stefan Sandfeld
IMFD/MiMM, TU Freiberg, Freiberg, Germany

12:00 **Machine learning a neural network magnesium potential**

Markus Stricker[1], Binglun Yin[1], Rasool Ahmad[1], Giulio Imbalzano[2], Michele Ceriotti[2], William Curtin[1]
[1]*Ecole Polytechnique Federale de Lausanne, Laboratory for Multiscale Mechanics Modeling, Lausanne, Vaud, Switzerland*
[2]*Ecole Polytechnique Federale de Lausanne, Laboratory for Computational Science and Modeling, Lausanne, Vaud, Switzerland*

12:15 **Extending the Peierls-Nabarro model using machine learning**

Amuthan Arunkumar Ramabathiran
Department of Aerospace Engineering, Indian Institute of Technology Bombay, Mumbai, Maharashtra, India

12:30-13:45 Lunch Break ***Dining Room***

13:45-19:00 Conference Tour to Akko (Acre)

13:45 Departure from the lobby of the Dan Panorama Hotel

THURSDAY, SEPTEMBER 19, 2019

09:00-10:30 Session 11 – Grain And Twin Boundaries (1) — Alon Hall

Chair: **Marc Legros,** CNRS, Toulouse, France

09:00 *Invited Lecture*

Grain Boundary Dynamics = Disconnection Dynamics

David Srolovitz[1,2], Jian Han[2], Kongtao Chen[2], Spencer Thomas[2,3]
[1]*Materials Science and Engineering, City University of Hong Kong, Kowloon, Hong Kong*
[2]*Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA, USA*
[3]*Materials Science and Engineering, North Carolina State University, Raleigh, NC, USA*

09:30 *Invited Lecture*

Modeling 3-D grain boundary evolution driven by the five-dimensional grain boundary energy landscape

Nikhil Chandra Admal[1], Javier Segurado[4], Matt Jacobs[3], Stanley Osher[3], Jaime Marian[2]
[1]*Department of Mechanical Science and Engineering, University of Illinois Urbana-Champaign, Urbana, IL, USA*
[2]*Department of Materials Science and Engineering, University of California Los Angeles, Los Angeles, CA, USA*
[3]*Department of Mathematics, University of California Los Angeles, Los Angeles, CA, USA*
[4]*IMDEA Materials Institute, Madrid, Spain*

10:00 *Invited Lecture*

On the role of interface structure, morphology and misfit stresses in dislocation-precipitate interactions

Erik Bitzek, Aviral Vaid, Frédéric Houllé, Hao Lyu
Department of Materials Science and Engineering, Institute I, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

10:30-11:00 Coffee Break

11:00-12:15 Session 12 – Grain and Twin Boundaries (2) — Alon Hall

Chair: **Christoph Kirchlechner,** Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

11:00 *Invited Lecture*

In situ TEM and simulation study of shear-migration coupling of grain boundaries

Marc Legros[1,2], Frédéric Mompiou[1,2], Armin Rajabzadeh[1], Romain Gautier[1,2,3], Melvyn Larranaga[1,2], Nicolas Combe[1,2]
[1]*CEMES, CNRS, Toulouse, France*
[2]*Université Paul Sabatier, Université de Toulouse, Toulouse, France*
[3]*Institut P Prime, Université de Poitiers, Poitiers, France*

11:30 **Investigation of the role of disconnections in the shear coupled grain boundary migration mechanism**

Melvyn Larranaga, Frederic Mompiou, Nicolas Combe, Marc Legros
CEMES-CNRS, Université Toulouse, Toulouse, France

11:45 **Kinetic laws for the motion of twin boundaries in ferroic materials: the role of twinning disconnections**

Eilon Faran, Doron Shilo
Department of Mechanical Engineering, Technion – Israel Institute of Technology, Haifa, Israel

12:00 **On interaction of twinning disconnections with obstacles in hcp metals**

Andrej Ostapovec
CEITEC-IPM, Institute of Physics of Materials ASCR, Brno, Czech Republic

12:15-13:45 Lunch Break — ***Dining Room***

13:45-15:15 Session 13 – Grain and Twin Boundaries (3) & Brittle-to-Ductile Transition — Alon Hall

Chair: **Erik Bitzek,** Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

13:45 *Invited Lecture*
Understanding dislocation twin boundary interactions: From single twin boundaries towards nanotwinned materials

Christoph Kirchlechner, Maya K. Kini, Nataliya V. Malyar, Juan Li, Gerhard Dehm
Structure and Nano-/Micromechanics, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

14:15 **Atomic simulations of dislocation interactions with coincidence site lattice boundaries in silicon**

Simen Nut Hansen Eliassen[1], Jesper Friis[2], Inga Ringdalen[2], Yanjun Li[1]
[1]*Department of Materials Science and Engineering, Norwegian University of Science and Technology, Trondheim, Norway*
[2]*Materials and Chemistry, SINTEF, Trondheim, Norway*

14:30 **Large scale 3D atomistic simulations of dislocation interactions with bicrystalline interfaces during multiaxial loading**

Maxime Dupraz[1,2], Satish I. Rao[3], Helena Van Swygenhoven[2,4]
[1]*CNRS IM2NP UMR 7334, Aix Marseille Univ, Marseille, France*
[2]*Swiss Light Source, SYN-PEM, Paul Scherrer Institut, Villigen, Switzerland*
[3]*Materials Directorate, Air Force Research Laboratory, Wright-Patterson Air Force Base, Ohio, USA*
[4]*NXMM-IMX-STI, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

14:45 **The Brittle to Ductile Transition and the core structures of dislocations in silicon**

Jacques Rabier
DPMM, Institut Pprime, UPR 3346 CNRS – Université de Poitiers –ENSMA, CNRS, Chasseneuil Futuroscope, France

15:00 **Kink-limited Orowan strengthening and the brittle to ductile transition of bcc metals**

Thomas Swinburne[1], Sergei L. Dudarev[2], Mihai-Cosmin Marinica[3]
[1]*CINaM, CNRS, Marseille, France*
[2]*Theory and Modelling of Materials, Culham Center for Fusion Energy, Oxford, UK*
[3]*SRMP, CEA, Saclay, France*

15:15-15:45 Coffee Break

15:45-16:45 Session 14 – Dislocations in Alloys — Alon Hall

Chair: **Alfonso Ngan,** University of Hong Kong, Pokfulam, Hong Kong

15:45 *Invited Lecture*
On the glide of [100] dislocation and the origin of "pencil glide" in Mg_2SiO_4 olivine: insights from atomic scale modeling

Philippe Carrez, Srinivasan Mahendran, Patrick Cordier
UMET Laboratory CNRS-UMR 8207, University of Lille, Villeneuve d'Ascq, France

16:15 **Dislocation mechanisms in TiAl during low cycle fatigue at 800°C investigated by TEM**

Soumaya Naanani[1,2], Alain Couret[1], Muriel Hantcherli[1], Catherine Mabru[2], **Jean-Philippe Monchoux**[1]
[1]*CEMES UPR 8011, CNRS, Toulouse, France*
[2]*ISAE, SUPAERO, Toulouse, France*

16:30 **Systematic investigation of the deformation mechanisms of a γ-TiAl single crystal**

Taegu Lee[1], Byungkwan Jeong[1], Jaemin Kim[1], Seong-Woong Kim[2], **Seunghwa Ryu**[1]
[1]*Mechanical Engineering, Korea Advanced Institute of Science and Technology, Daejeon, South Korea*
[2]*Titanium Department, Korea Institute of Materials Science, Changwon, South Korea*

16:45-18:15 Free Time

18:15 - Departure to the Technion from the Dan Panorama Hotel

19:00-20:00 Keynote Lecture — Technion (Dan-Kahn Bldg., Hall 6)

Dan Shechtman, Nobel Prize Laureate in Chemistry 2011
Department of Maretials Science and Engineering, Technion – Israel Institute of Technology, Haifa, Israell

20:00-22:00 CONFERENCE DINNER — *Technion (Dan-Kahn Bldg.)*

Return transportation to the conference hotels, will be provided after dinner.

FRIDAY, SEPTEMBER 20, 2019

09:00-10:45 Session 15 – Dislocations in Nanostructures (1) Alon Hall

Chair: **Eugen Rabkin,** Technion – Israel Institute of Technology, Haifa, Israel

09:00 *Invited Lecture*
3D imaging of dislocations with x-rays: recent trends and future prospects

Olivier Thomas[1], Thomas Cornelius[1], Marie-Ingrid Richard[1,2], Stephane Labat[1], Florian Lauraux[1], Jérome Carnis[1,2], Maxime Dupraz[1,2]
[1]*Aix Marseille Univ, CNRS IM2NP UMR 7334, Marseille, France*
[2]*ESRF, ID01, Grenoble, France*

09:30 **Geometrically necessary dislocations in three-point bent Au nanowires studied by in-situ Laue microdiffraction**

Thomas Cornelius[1], Zhe Ren[1], Odile Robach[2,3], Jean-Sébastien Micha[2,3], Gunther Richter[4], Olivier Thomas[1]
[1]*IM2NP, Aix Marseille Univ, Univ de Toulon, CNRS, Marseille, France*
[2]*CRG-IF BM32 Beamline, European Synchrotron (ESRF), Grenoble, France*
[3]*CEA/INAC, Université Grenoble Alpes, Grenoble, France*
[4]*Intelligent Systems, Max Planck Institute, Stuttgart, Germany*

09:45 **In situ transmission electron microscopy observations of the fcc-hcp phase transformation in Co nanowhiskers**

Gunther Richter, Wenting Huang
ZWE Materials, Max Planck Institute for Intelligent Systems, Stuttgart, Germany

10:00 *Invited Lecture*
The stochastics of strain localization in metallic-glass microwires

Alfonso Ngan[1], Kefu Gan[1], S.S. Jiang[2], H.B.C. Yin[2], Y.J. Huang[2]
[1]*Department of Mechanical Engineering, University of Hong Kong, Pokfulam, Hong Kong*
[2]*School of Materials Science and Engineering, Harbin Institute of Technology, Harbin, Heilongjiang, China*

10:30 **Stochastic behavior of dislocation nucleation from acute and obtuse angles in metallic nanowires**

Stav Nisany, Tomer Gur-Apter, **Dan Mordehai**
Department of Mechanical Engineering, Technion – Israel Institute of Technology, Haifa, Israel

10:45-11:15 Coffee Break

FRIDAY, SEPTEMBER 20, 2019

11:15-12:30 Session 16 – Dislocations in Nanostructures (2) — Alon Hall

Chair: **Dan Mordehai,** Technion – Israel Institute of Technology, Haifa, Israel

11:15 Effect of solute atoms and Peierls stress on the critical behaviour of dislocations

Peter Ispanovity[1], Gábor Péterffy[1], Peter M. Derlet[2]
[1]*Department of Materials Physics, Eotvos University, Budapest, Hungary*
[2]*Condensed Matter Theory Group, Paul Scherrer Institut, PSI-Villigen, Switzerland*

11:30 Nucleation and structure of Van der Waals dislocations in 2D materials

Harley Johnson[1], Shuze Zhu[1], Emil Annevelink[1], Pascal Pochet[2]
[1]*Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL, USA*
[2]*INAC Laboratory for Atomistic Simulation, CEA-Grenoble & Universite Grenoble-Alpes, Grenoble, France*

11:45 Atomistic simulations of stress/strain maps of alloyed nanoparticles

Christine Mottet, Alexis Front
CINaM - CNRS/AMU, CNRS, Marseille, France

12:00 Record-breaking strength and solid solution softening in Ni and Ni_3Fe nanoparticles

Amit Sharma[1], James Hickman[2], Oz Mendelsohn[1], Nimrod Gazit[1], Yuri Mishin[2], **Eugen Rabkin**[1]
[1]*Department of Materials Science and Engineering, Technion – Israel Institute of Technology, Haifa, Israel*
[2]*Department of Physics and Astronomy, George Mason University, Fairfax, VA, USA*

12:15 Three-dimensional structural imaging of defects in Pt nanocrystals

Marie-Ingrid Richard[1], Jérome Carnis[1], Maxime Dupraz[1], Stephane Labat[1], Lu Gao[2], Jan Philipp Hofmann[2], Nimrod Gazit[3], Eugen Rabkin[3], Emiel Hensen[2], Tobias Schulli[4], Olivier Thomas[1]
[1]*Physics Department, IM2NP-CNRS 7334, Aix Marseille University, Marseille, France*
[2]*Inorganic Materials & Catalysis, Eindhoven University of Technology, Eindhoven, Netherlands*
[3]*Materials Science and Engineering, Technion Israel Institute of Technology, Haifa, Israel*
[4]*Experimental division, The European Synchrotron, Grenoble, France*

12:30-12:45 Closing Remarks — Alon Hall

12:45-13:30 Light Lunch

TUESDAY, SEPTEMBER 17, 2019

20:00-22:00 POSTER VIEWING SESSION (wine & beer) Pythagoras Hall

P-1 A continuum non-singular theory of thermally fluctuating dislocations

Max Boleininger[1], Thomas Swinburne[2], Sergei L. Dudarev[1]
[1]*Materials Modelling Group, Culham Centre for Fusion Energy, Abingdon, Oxfordshire, UK*
[2]*Centre Interdisciplinaire des Nanosciences de Marseille, Aix-Marseille Univ.-CNRS, Marseille, France*

P-2 Molybdenum plastic deformation: From large scale molecular dynamics simulations towards continuum dislocation dynamics

Pavel Pokatashkin, Alexei Yanilkin
Materials Science Division, Dukhov Research Institute of Automatics, Moscow, Russia

P-3 Analysis of austenite-martensite phase boundary and twinned microstructure in shape memory alloys: The role of twinning disconnections

Emil Bronstein, Eilon Faran, **Doron Shilo**
Department of Mechanical Engineering, Technion – Israel Institute of Technology, Haifa, Israel

P-4 An effective implicit method for discrete dislocation dynamics simulation

Gábor Péterffy, Peter Ispanovity
Department of Materials Physics, Eötvös Loránd University, Budapest, Hungary

P-5 Observation of diffusion induced dislocations on single Crystalline Au nanowhiskers during interdiffusion studies

Eylul Suadiye[1], Yuanshen Qi[2], Eugen Rabkin[2], Gunther Richter[1]
[1]*Modern Magnetic Systems, Max Planck Institute for Intelligent Systems, Stuttgart, Germany*
[2]*Department of Materials Science and Engineering, Technion – Israel Institute of Technology, Haifa, Israel*

P-6 Critical examination of continuum and cross-core theories of dynamic strain aging

Ryan Sills, Ethan Epperly
Gas Transfer Systems, Sandia National Laboratories, Livermore, CA, USA

P-7 Acoustic emission in micropillar deformation experiments

Dávid Ugi[1], Péter Dusán Ispánovity[1], Krisztián Máthis[2], Michal Knapek[2], Istvan Groma[1], Zoltán Dankházi[1]
[1]*Department of Materials Physics, Loránd Eötvös University, Budapest, Hungary*
[2]*Department of Physics of Materials, Charles University, Prague, Czech Republic*

P-8 The Interplay between Dislocation Nucleation and Glide in the origin of the Hugoniot Elastic Limit Spike and Precursor Decay

Roman Kositski, Dan Mordehai
Department of Mechanical Engineering, Technion – Israel Institute of Technology, Haifa, Israel

P-9 **c+a dislocation glide in zirconium**

Thomas Soyez[1], Clouet Emmanuel[1], Fabien Onimus[2]
[1]*DANS/DEN/DMN/SRMP, Cea Saclay, Gif sur Yvette, France*
[2]*DANS/DEN/DMN/SRMA/LA2M, Cea Saclay, Gif sur Yvette, France*

P-10 **Stress-Dependent activation energy barrier for Cross-Slip in FCC metals**

Alon Malka-Markovitz, Dan Mordehai
Mechanical Engineering, Technion – Israel Institute of Technology, Haifa, Israel

P-11 **Influence of dislocations and Cottrell atmospheres on pressure-induced transformations in single-crystalline iron**

Hoang-Thien Luu[1], Nina Gunkelmann[1], Roberto G. A. Veiga[2]
[1]*Computational Material Sciences/Engineering, Institute of Applied Mechanics, Clausthal University of Technology, Clausthal-Zellerfeld, Germany*
[2]*Center of Engineering, Modeling and Applied Social Sciences, Federal University of ABC, São Paulo, Brazil*

P-12 **A microstructural perspective on the dynamic stored energy of cold work**

Juan Carlos Nieto-Fuentes, Daniel Rittel, Shmuel Osovski
Faculty of Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel

P-13 **Stable networks containing two pieswise dislocation arrays**

Roni Z. Shneck, Nitzan Mizrahi
Materials Engineering, Ben Gurion University of the Negev, Beer Sheva, Israel

P-14 **Screw dislocation-carbon interaction in BCC tungsten: An *ab initio* study**

Guillaume Hachet, Emmanuel Clouet, Lisa Ventelon
DEN - Service De Recherches De Métallurgie Physique, CEA- Saclay, Gif-sur-Yvette, France

P-15 **Compression of Nanoporous Au Nanopillars in Molecular Dynamics Simulations**

Santhosh Mathesan, Dan Mordehai
Department of Mechanical Engineering, Technion-Israel Institute of Technology, Haifa, Israel

P-16 **Compression Strength of Ni-Fe Nanoparticles**

Oz Mendelsohn[1], Eugen Rabkin[1], Yuri Mishin[2]
[1]*Department of Material Science and Engineering, Technion – Israel Institute of Technology, Haifa, Israel*
[2]*Department of Physics and Astronomy, George Mason University, Fairfax, VA, USA*

ABSTRACTS

Oral Presentations

Session 1 – Dislocation-solute interaction (1)
(Monday, September 16, 2019 09:15)

Invited lecture

Invited Lecture

Dislocations and strengthening in random BCC alloys

William Curtin, F. Maresca
Mechanical Engineering, EPFL, Lausanne, Switzerland

BCC High Entropy Alloys (HEAs) consist of many elements distributed at random on the BCC lattice. The collective fluctuations in solute/dislocation interaction energies, even in dilute binary BCC alloys, lead to the spontaneous energy-lowering formation of a kinked/wavy structure for both screw and edge dislocations, respectively, over characteristic lengths $\zeta_{c,screw}$ and $\zeta_{c,edge}$. Dislocation motion starting from the kinked/wavy structure is determined by the energetics at scale ζ_c. New general theories for both screw and edge motion in BCC alloys starting from this basic phenomenon are presented. The screw theory is sketched briefly, and shown to accurately predict strength versus composition and temperature in Nb-Mo and Nb-W binary alloys. As for BCC elements, the necessary inputs are difficult to establish, especially in more complex alloys. Key comparisons to simulations help demonstrate major features of the theory. Most unusual is that edge strengthening can be sufficient to compete with screw strengthening. Moreover, edges can control strengthening, especially at high temperatures, in some BCC HEAs. The edge theory, for which all inputs can be computed easily, explains (i) the exceptional retention of strength measured in MoNbTaW and MoNbTaVW at temperatures up to 1900K, and (ii) why the V-containing alloy is stronger. The edge theory can be reduced to a simplified analytic form that enables efficient computationally-guided design of new alloy compositions predicted to have high retained strengths and strength-to-weight ratios. Several new compositions are proposed [2]. The combination of both screw and edge theories enables assessment of strengthening versus composition and temperature across the entire domain of Cr-Mo-Nb-Ta-V-W-Hf-Ti-Zr BCC HEAs.

Invited lecture

Invited Lecture

Simulating dislocation-solute co-evolution in body-centered cubic metals on diffusive timescales

Yue Zhao[1], Lucile Dezerald[2], **Jaime Marian**[1]
[1]*Materials Science and Engineering, UCLA, Los Angeles, CA, USA*
[2]*Institut Jean Lamour, Université de Lorraine, Nancy, France*

The interaction between solute atoms and dislocations is behind numerous mechanical behavior processes of great importance in materials science. In addition to solution hardening and/or softening, solutes may also dynamically evolve around dislocation cores, giving rise to important phenomena such as the formation of solute clouds, jerky flow, dynamic strain aging, etc. Typically, dislocation-solute interactions are modeled in the two extremes of the adiabatic approximation where either dislocations or solutes are stationary on the timescale of motion of the other. While this can give insight into processes such as solid solution strengthening or solute could formation, it cannot capture dynamic effects where both subpopulations evolve on comparable timescales. In addition, in body-centered cubic alloys, plastic flow is generally controlled by the thermally activated motion of screw dislocations, which proceeds by nucleation and propagation of kinks along the dislocation line. As such, solute-dislocation interactions must be dealt with in a manner consistent with this intrinsic behavior. In this work, we present a kinetic Monte Carlo model where solute hopping and kink-pair nucleation/motion are part of a unified framework where both subspecies evolve concurrently and are coupled by bidirectional elastic and inelastic interactions. The coupling is done by calculating the elastic dipole tensors using electronic structure calculations, as well as by obtaining inelastic interaction energies between dislocation cores and solute atoms. We use the parameterized model to predict the hardening-softening transition in W-Re alloys and to capture the conditions under which dynamic strain aging might be expected in W-O alloys.

Oral presentation

Large-scale molecular dynamics simulations reveal length-dependent dislocation mobilities in Fe-Cr-Ni austenitic stainless steel

Ryan Sills[1], Michael Foster[2], Xiaowang Zhou[2]
[1]*Gas Transfer Systems, Sandia National Laboratories, Livermore, CA, USA*
[2]*Mechanics of Materials, Sandia National Laboratories, Livermore, CA, USA*

We present a systematic study of edge dislocation mobility in random, austenitic $Fe_{0.7}Ni_{0.11}Cr_{0.19}$ alloys over a range of temperatures, stresses, and dislocation line lengths. Our results reveal that, below a minimum dislocation line length, solid solution strengthening is intrinsically line-length-dependent. Below the minimum length, the dislocation mobility is reduced and strengthening is increased. We show that the minimum line length is both stress- and temperature-dependent, and anticipate that it is also sensitive to solute type and concentration. Furthermore, analysis of the dislocation line configurations in the solute drag regime reveals that dislocation lines adopt large amplitude (50), wavy configurations during glide. Our findings present evidence that the characteristic segment length invoked by the recent solute strengthening model of Leyson and Curtin (LC) is a real feature of dislocation-solute interactions. Using solute, phonon, and wave-speed-induced drag parameters extracted from the MD data, we develop a kinetic Monte Carlo (kMC) model inspired by the LC model that rationalizes the length dependence of the mobility. The kMC model cannot reproduce the large bowing that is observed in the MD simulations, however, unless the dislocation line tension adopts unphysically small values.

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Invited lecture

Invited Lecture
Multiscale modelling of precipitation hardening in metallic alloys

Javier LLorca
IMDEA Materials Institute & Polytechnic University of Madrid, Madrid, Spain

Precipitation hardening is one of the most efficient mechanisms to increase the yield strength of metallic alloys but accurate quantitative models for this phenomenon are still lacking. Two different multiscale approaches, based on atomistic simulations and discrete dislocation dynamics, are presented to address this problem and validated by comparison with experiments.

Atomistic simulations were used to determine the interaction between Guinier-Preston zones and dislocations in an Al-Cu alloy. The rate at which dislocations sheared the precipitates (determined by means of molecular dynamics) was controlled by the activation free energy, in agreement with the postulates of the transition state theory. An estimation of the initial shear flow stress as a function of temperature was carried out from the thermodynamic data provided by the atomistic simulations.

In the case of large precipitates that cannot be sheared by dislocations (such as θ' precipitates in Al-Cu alloy), the dislocations overcome the precipitates by the formation of an Orowan loop. The mechanisms of dislocation/precipitate interaction were studied by means of discrete dislocation dynamics using the discrete-continuous method in combination with a fast Fourier transform solver to compute the mechanical fields. Simulations took into account the effect of precipitate shape, orientation and volume fraction as well the elastic mismatch between the matrix and the precipitate, the stress-free transformation strain around the precipitate and the dislocation character as well as dislocation cross-slip. The simulation predictions were compared with experimental results of the initial yield strength in an Al-Cu alloy overaged at high temperature.

Oral presentation

Plasticity and dislocation mechanisms in aluminium alloys containing precipitate free zones

Inga Ringdalen[1], Sigurd Wenner[1], Jesper Friis[1], Emil Christiansen[2,3], Jonas Frafjord[2,3], Mikhail Khadyko[4], Odd Sture Hopperstad[2,4], Randi Holmestad[2,3]
[1]*Department of Materials and Nanotechnology, Sintef Industry, Trondheim, Norway*
[2]*Centre for Advanced Structural Analysis (CASA), Norwegian University of Science and Technology, Trondheim, Norway*
[3]*Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway*
[4]*Department of Structural Engineering, Norwegian University of Science and Technology, Trondheim, Norway*

Age hardening of commercial Al-Mg-Si aluminium alloys results in microstructures characterized by needle-shaped Mg- and Si-rich precipitates. At peak strength, the most prominent of these is the non-equilibrium β`` phase. This precipitate are coherent with the fcc Al lattice, and can cause considerable hardening by restricting dislocation movement. Precipitate free (denuded) zones, with no or a very limited amount of strengthening precipitates, are formed around grain boundaries after the solution heat treatment. The width of these zones is around 100-500 nm depending on cooling rate and alloy composition. They strongly influence the global mechanical properties of the alloy due to strain localization and following ductile fracture initiated within or close to these zones. To understand the influence of precipitate free zones on the global material behaviour, a detailed understanding of the local plasticity and dislocation mechanisms is necessary. Aluminium alloys containing precipitate free zones have therefore been studied by modelling and simulations, ranging from crystal plasticity to molecular dynamics, and experiments using nanohardness measurement and transmission electron microscopy.

Oral presentation

Atomistic phase field chemomechanical modeling of defect-solute interaction in metallic alloys

Bob Svendsen[1,3], Jaber Rezaei Mianroodi[1,3], Pratheek Shanthraj[2]
[1]*Material Mechanics, RWTH Aachen University, Aachen, Germany*
[2]*School of Materials, University of Manchester, Manchester, UK*
[3]*Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany*

The interplay between chemistry and defects is important in determining the material behavior of many engineering alloys. Spatial fluctuations in chemical composition result in heterogeneous material properties affecting in particular defect formation and evolution. In addition, the difference between defect and bulk thermodynamics results in chemical partitioning between these. Given its energy basis, phase field (PF) modeling combined with mechanical defect modeling is ideally suited to study this strong two-way coupling between chemistry and defect evolution. In the current model, large-deformation-based mechanical equilibrium is coupled with PF modeling of defects and chemistry. In particular, the model accounts for elastic anisotropy, concentration dependent stiffness, solute residual distortion, and the concentration dependence of defect and stacking fault energies. In addition, Cahn-Hilliard modeling of solute concentration is coupled with Ginzburg-Landau modeling of defect evolution. Particular defects considered here include dislocations, precipitates, and low angle grain boundaries. The entire energy model is calibrated using atomistic and / or CALPHAD information (in the latter case, for solute mobility and chemical energy). This ensures for example accurate treatment of core size and dislocation transformation pathways. A number of example simulations and comparison with experimental results from atom probe tomography and transmission electron microscopy will be given.

Oral presentation

The effect of multiple species in solute strengthening in aluminium – A molecular dynamics study

Jonas Frafjord[1,4], Jesper Friis[2,4], Randi Holmestad[1,4], Bjørn Holmedal[3], Inga Ringdalen[2,4]
[1]*Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway*
[2]*Industry, SINTEF, Trondheim, Norway*
[3]*Department of Materials Science and Engineering, Norwegian University of Science and Technology, Trondheim, Norway*
[4]*NA, SFI Center for Advanced Structural Analysis, Trondheim, Norway*

The strength of a metallic alloy is controlled by the collective contribution from different strengthening mechanisms. To develop a complete numerical framework for the flow stress in alloys, it is necessary to understand the different mechanisms isolated, as well as knowing how they interact and affect each other. Several models for the solute strengthening contribution based on first principle calculations have been developed in the recent years [1,2]. These models have treated single solute species and predicted flow stress in good agreement with experimental results. The effect of multiple species has not yet been investigated with the same level of complexity, resulting in a lack of understanding of solute strengthening. The effect of multiple solute species is often a source of error in higher scale strengthening models, where the effective contribution from solute strengthening is calculated by a linear combination of the different species, or scaled by an effective concentration.

In this work, we have conducted a molecular dynamics study of an aluminium alloy with a random distribution of silicon and magnesium solutes. The simulations are combined with an analytical study of the isolated systems with a single solute species and a mobile dislocation. Models used to calculate the solute strengthening contribution at higher length scales are investigated, as an attempt to validate their approach. The empirical parameters used in these models are calculated by molecular dynamics. In addition, the study aims to broaden the understanding of dislocation bow out, and how it affects the mobility of dislocations.

[1]:https://doi.org/10.1016/j.actamat.2016.09.046

[2]:https://doi.org/10.1038/nmat2813

Invited lecture

Invited Lecture

Mobility of screw dislocations in hexagonal close-packed zirconium and titanium

Emmanuel Clouet[1], Nermine Chaari[1], David Rodney[2], Daniel Caillard[3]
[1]*SRMP, CEA Saclay, Gif-syr-Yvette, France*
[2]*ILM, Université Lyon 1 / CNRS, Lyon, France*
[3]*CEMES, CNRS, Toulouse, France*

Titanium and zirconium have a close plastic behaviour arising from their hexagonal close-packed crystallography and from their similar electronic structure. In particular, plasticity in these two transition metals is controlled by screw dislocations gliding in the prism planes, with cross-slip in the first-order pyramidal planes or in the basal planes activated at high enough temperature and a strong hardening associated with interstitial solute addition. We use atomistic simulations relying on ab initio calculations to study core properties of the screw dislocations and their mobility in both metals. These calculations show that screw dislocations may adopt different cores that are dissociated either in a prism or in a pyramidal plane. The prismatic core easily glides in its habit plane, whereas the pyramidal core needs to overcome an important energy barrier to glide. The prismatic glissile core is the most stable in Zr, but the dislocation ground state in Ti corresponds to the pyramidal core. As a consequence, dislocation glide is easy and confined in the prismatic planes at low temperature in pure Zr, whereas a locking-unlocking mechanism operates in Ti where the locked periods correspond to a slow and limited glide in pyramidal planes and the unlocked periods to a rapid and extended glide in prismatic planes, in agreement with in situ TEM straining experiments. Finally, we study the interaction of interstitial solute atoms, in particular oxygen and sulfur, with these different configurations of the screw dislocation. Ab initio calculations evidence a strong repulsion with both solutes repelling the stacking fault ribbon, thus inducing dislocation cross-slip and leading to the production of jogs on the screw dislocation. This short-range interaction mechanism is responsible for the strong hardening associated with oxygen addition.

Oral presentation

Invited Lecture

Non-Schmid effects in BCC metals from first principles

Lucile Dezerald[1,2], Antoine Kraych[3], Bassem Ben Yahia[1,2], Emmanuel Clouet[4], Lisa Ventelon[4], François Willaime[5], David Rodney[3]
[1]*Institut Jean Lamour, Université de Lorraine, Nancy, France*
[2]*LabEx DAMAS, Université de Lorraine, Metz, France*
[3]*Institut Lumière Matière, Université Lyon 1, Villeurbanne, France*
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Body-centered cubic (BCC) metals are known for their atypical plasticity at low temperatures. Here, we focus on their plastic anisotropy and dependence on non-glide stresses, which contradict Schmid's law. Plasticity of BCC metals is controlled by the glide of ½ screw dislocations. These dislocations display strong core effects at the atomic scale that are responsible for the atypical low temperature plasticity. Here, we use ab initio Density Functional Theory calculations to investigate the link between the core properties of the screw dislocations and deviations from Schmid's law in BCC metals. We find that the dislocation trajectory systematically deviates from the average glide plane, leading to the well-known twinning/antitwinning asymmetry [1]. Furthermore, we show that the dislocation core deformation modeled with eigenstrains is directly linked to the effect of non-glide stresses. In particular, core eigenstrains measured in absence of applied stress enable to predict the hardening and softening of the Peierls barrier when the glide plane is either under compression or tension. These results are used in a modified version of Schmid's law in order to predict the variations of the critical resolved shear stress (RSS) as a function of crystal orientation and non-glide stresses [2]. We evidence a strong twinning/antitwinning and tension/compression asymmetry of the critical RSS, directly linked to the dislocation trajectory and eigenstrain variations at the atomic scale. These results are validated by comparison with direct DFT calculations performed under shear and non-glide stresses.

[1] Dezerald et al, Nature Communications 7, 11695 (2016)

[2] Kraych et al, submitted to NPG Computational Materials

Oral presentation

Origin of anomalous slip in bcc metals

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The anomalous slip, first observed by Duesbery and Foxall in Nb (Phil. Mag. A 20:719, 1969), is the slip along the {110}111 system with very low Schmid factor that dominates straining at low temperatures. Since then, this phenomenon has been observed in several transition bcc metals but not in all, notably not in alpha-Fe. In 1973, Matsui and Kimura proposed a "co-planar double slip" model to explain the anomalous slip when considering the glide of 1/2[111] and 1/2[-111] screw dislocations on the (0-11) plane. This model is based on the assumption that the two intersecting screw dislocations and the associated 100 screw junction form a dislocation network, which can only move on the (0-11) plane. We have made a series of molecular statics simulations employing bond order potentials to investigate the glide of these junctions in five non-magnetic bcc refractory metals (Ta, Nb, V, Mo, W) and alpha-Fe. The external load was applied as uniform uniaxial tension and compression in the [-238] direction for which the (-101) plane is the maximum resolved shear stress plane for the 1/2[111] dislocation. Two different behaviors of this network are observed depending on the material and the character of the applied load. In some materials, the three dislocations move on the low-stressed (0-11) plane, in agreement with the predictions of the model of Matsui and Kimura. However, in other materials, the two 1/2111 dislocations break from the junction and move on their expected {110} planes. In the latter case, no anomalous slip occurs. These observations suggest that the anomalous slip is not generic for transition metals and its occurrence depends on details of bonding controlled by the electronic structure.

Oral presentation

Effect of solutes on the core structure and mobility of dislocations in bcc metals

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The interaction between interstitial solute atoms and screw dislocations was studied in several body centered cubic metals using electronic structure calculations based on the Density Functional Theory (DFT). In a first step, considering carbon solutes, we have evidenced a strongly attractive interaction in Fe, Mo and W, induced by a spontaneous reconstruction of the core structure towards a low energy configuration where, unexpectedly, the dislocation core adopts a hard-core configuration. The carbon atoms are at the center of regular trigonal prisms formed by the metal atoms in the dislocation core. The preference of carbon atoms for these prismatic sites can be related to the similarity with their local environment in Fe3C cementite and in WC and MoC hexagonal carbides. We have evidenced the same core reconstruction with other octahedral interstitial solutes (B, N, O) in Fe, whereas a totally different behavior is obtained for the carbon in V, Nb and Ta. We show, using a thermodynamic model, that this highly attractive interaction leads to complex segregation phenomena with a dislocation core fully saturated by solute atoms at low temperature even for very low bulk carbon concentrations. Finally, we investigated the consequences on the mobility of dislocations in Fe (C) based on the DFT calculations of the kink-pair formation and kink migration on decorated dislocations.

Oral presentation

Core structure and mobility of mixed ½ [111] dislocations in bcc metals

Tapaswani Pradhan[1], Anastasiia Kholtobina[2], **Lorenz Romaner**[2], Matous Mrovec[1], Ralf Drautz[1]

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The body-centered cubic metals represent a technologically highly relevant material class including Fe and the refractory metals W and Mo. A major drawback of this material class is given by the brittle-to-ductile transition which for some metals, e.g. W occurs above room temperature. A dominant role in this connection is assigned to the ½ screw dislocation which, due to a non-planar core, has low mobility and limits plastic deformation. However, it has been proposed recently that mixed ½ dislocations, which are of predominantly edge character and therefore expected to be glissile, possess unexpectedly high Peierls stress. Therefore, such dislocations might play an equally important role for the limited plastic deformation at low temperature. So far the issue has not been systematically investigated for the class of bcc transition metals Nb, Ta, Mo, W and Fe.

In this study, we investigate the core structures and mobilities of mixed ½ dislocations in five BCC transition elements Nb, Ta, Mo, W and Fe using atomistic simulations. The simulations were carried out with different models of interatomic interactions, ranging from classical potentials via tight-binding-based bond order potentials to first-principles methods based on density functional theory. We find pronounced differences for the structure of the dislocation core in terms of width and dissociation into fractionals. As a result, Peierls barriers vary strongly between the different transition metals. By comparing mobility of the mixed dislocation with the one of the screw dislocation we provide hints to what extent mixed dislocations matter in the different metals and discuss the implications of our findings for thermal activation of dislocation glide and shape of dislocation loops.

Oral presentation

Atomistic simulations of dislocations in iron-chromium alloys

Matous Mrovec, Sergei Starikov, Ralf Drautz
ICAMS, Ruhr-Universität Bochum, Bochum, Germany

Dislocations in bcc metals exhibit large differences in their mobilities. While pure screw dislocations experience high lattice resistance due to their non-planar cores, all non-screw dislocations are expected to glide easily at low applied stresses. However, dislocation properties can change significantly in alloys due to different chemical bonding and size mismatch of the constituting elements.

In this work, we investigate properties of dislocations in the Fe-Cr system that is both technologically important and scientifically challenging since many structural, mechanical and thermodynamic properties of this system are governed by magnetic interactions. To obtain a comprehensive picture, we employ a range of atomistic methods including first-principles calculations, tight binding and related magnetic bond-order potentials, as well as classical interatomic potentials. We will present an analysis of both static (structural, magnetic) and dynamic (behavior under applied stress) properties of dislocations for various Fe-Cr compositions and discuss the implications on the plastic behavior.

Oral presentation

Plastic deformation of chromium single crystals at 77 K

Jakub Holzer[1], Roman Gröger[1], Zdeněk Chlup[2]
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[2]*Department of Brittle Fracture, Institute of Physics of Materials of Czech Academy of Sciences, Brno, Czech Republic*

Chromium (Cr) is an antiferromagnetic body-centered cubic (bcc) metal with longitudinally polarized spin density waves below 123 K. Virtually nothing is known about the plastic deformation its single crystals and the changes of internal magnetic order around extended defects such as dislocations. The present study provides for the first time a detailed analysis of deformation mechanisms operative in macroscopic single crystals of Cr with 99.999% purity. Samples with different orientations are compressed at 77 K to 2-4% of plastic strain at strain rates around 10^{-5} s^{-1}. The slip trace analysis is made by light microscopy using the Normarski differential interference contrast, more detailed investigations of slip morphology is made by the scanning electron microscopy in conjunction with the electron backscatter diffraction technique to determine sample orientation before/after deformation. The experimental results are reconciled using the theoretical predictions made by an effective yield criterion for Cr that was developed recently using molecular statics studies of an isolated 1/2[111] screw dislocation under stress.

Invited lecture

Invited Lecture

Linear complexion formation driven by local stress concentrations near dislocations

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Grain boundary complexions (phase-like interfacial structures) have been a major new area of exciting research. Analogous distinct structural states should also be possible at other types of defects such as dislocations, with recent experimental evidence of such features emerging from studies of Fe-Mn. In this work, we use atomistic modeling to study segregation and linear complexion formation along edge dislocations in both body-centered cubic and face-centered cubic metallic alloys. The local stresses associated with the dislocation can drive preferential segregation and local phase transformations, usually in the form of arrays of nanoscale precipitates. In Fe-Ni, we find that these precipitates are a combination of metastable B2-FeNi and stable $L1_0$-FeNi phases. For face-centered cubic metals, similar stress-driven segregation can occur but certain systems can also demonstrate segregation along the stacking fault between dissociated partial dislocations. For example, Cu-Zr can sustain a planar structure along the stacking fault that is reminiscent of the (111) plane of Cu_5Zr. For all of these alloys, we map out composition and temperature space to formulate “linear complexion phase diagrams” that will serve to guide future processing studies. Finally, we explore how these linear complexions affect the movement of dislocations, with an eye toward manipulating strength and strain hardening.

Invited lecture

Invited Lecture

Thermal fluctuations of dislocations

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Thermal fluctuations of dislocations control their mobility and set the time-scale of thermally activated events such obstacles by-pass or kink-pair nucleation. While dislocation vibrations have been previously investigated using simplified line tension descriptions and numerical dislocation dynamics (DD) models, we analyze them by the means of an analytical approach combined with atomistic simulations. Within the framework of the non-singular dislocation theory, we derived an analytical expression for the elastic energy of a weakly perturbed dislocation, which controls the amplitude of the equilibrium thermal fluctuations through the equi-partition theorem. Comparing this analytical prediction with molecular dynamics calculations performed in aluminum shows that a core energy (proportional to the dislocation length) has to be incorporated in addition to long-range elasticity. Adding this contribution allows to reproduce very accurately the fluctuation spectra obtained from molecular dynamics simulations over a large range of wave-vectors and yields quantitative estimates for the core parameter of the non-singular theory and for the magnitude of the core energy. We show that these parameters can be used in a higher scale DD model to reproduce accurately the dislocation behavior on short length-scales. Also, a deeper analysis of the time-dependence of the fluctuations yields valuable insights on the dynamical behavior of dislocations. Finally, we will discuss the transferability of our approach to high entropy alloys where a structural noise adds up to the thermal noise.

Oral presentation

Fundamental reactions between prismatic loops in stochastic dislocation dynamics

Max Boleininger[2], Yang Li[1], Christian Robertson[1], Laurent Dupuy[1], Sergei L. Dudarev[2]
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Body-centred cubic metals exposed to irradiation by energetic particles form highly mobile prismatic loops of 111 type, that in many cases represent the dominant type of radiation defects. As the microstructure of materials in a fusion reactor is expected to coarsen and evolve significantly over the service lifespan, one of the desired outcomes of fusion materials research is predicting the fundamental laws of evolution governing this process.

By virtue of their high mobility, prismatic loops often assemble into mutually trapped loop rafts at lower temperatures, while separating and dispersing at higher temperatures, with consequences to the mean obstacle distance and thus plasticity. The stochastic motion of individual loops and interacting clusters of loops, including reactions between the loops, is one of the central questions that needs resolving to enable the simulation of microstructure driven by stochastic forces associated with ambient thermal fluctuations. We find that the stochastic thermal force in conjunction with internal degrees of freedom, and the re-orientation of the loop habit-planes, is a factor fundamentally affecting the dynamics of interacting dislocation loops. The trapping reaction between the loops depends critically on the internal re-orientation of the loop habit plane during the reaction: the barrier to enter the bound state is lowered substantially to nearly athermal level, whereas the lifetime of the collective bound state is increased by several orders of magnitude.

In conclusion, we find that even within the simple (but elegant) theory of linear elasticity, the inclusion of internal degrees of freedom makes the fundamental difference between loop rafts remaining bound and stable, or separating on the experimentally relevant timescales.

Oral presentation

A molecular-dynamics investigation of single dislocations

Eyal Oren[1], Eyal Yahel[2], Guy Makov[1]
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[2]*Physics Department, NRCN, Beer-Sheva, Israel*

The kinematics and kinetics of edge and screw dislocations in FCC materials were studied by molecular dynamics (MD) simulations. In the first part, dislocations in single crystal Cu were accelerated to steady state velocities upon applying shear stress. It was found that screw dislocations enter into the transonic regime continuously with increasing stress. Edge dislocations were limited by the lowest transverse sound velocity (ca. 1.6 km/s) at low stresses and discontinuously crossed into the transonic regime at higher stresses. For sufficiently long edge dislocations the subsonic-transonic transition was initiated by an athermal nucleation process. Finally the velocity dependence of the dislocation mobility was derived. In the second part the kinetics of cross-slip and annihilation of a screw dislocation dipole in Cu, Al, and Ni were studied by multiple MD simulations of long (200b) dislocations at selected stresses and temperatures with the aim to account for the thermally activated nature of the cross-slip process. The cross- slip mechanism that was identified required the formation of a finite length constriction before cross-slip could be initiated. It was shown that point constrictions are not the transition state of cross-slip. The long dislocations in this study allowed multiple cross-slip events to occur independently along the dislocation line, leading to termination of the cross-slip process by formation of sessile loops. A study of the kinetics confirmed that cross-slip is a first-order process. The generated statistical data allowed the calculation of cross-slip activation energy and volume.

Oral presentation

Atomistic simulation of jog pair in magnesium oxide

Jian-Hui Zhai, Pierre Hirel, Philippe Carrez
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Magnesium oxide MgO is known for its ductility, allowed by dislocations which are surprizingly glissile for an oxide ceramic material. However in high-temperature applications, the enhanced diffusion may activate another mechanism: dislocation climb, where a dislocation moves out of its glide plane. This is particularly true when one considers creep conditions, where high temperatures come together with very slow strain rates.

In this work, we investigate dislocation climb in magnesium oxide for the two main slip systems [110](110) by means of atomistic simulation. The edge dislocation core configurations are obtained at different pressuresfrom dislocation dipolar configurations with periodic boundary conditions. Jog pair configurations are constructed by duplicating different dislocation dipole configurations. We determine the formation energy of jog pairs under various pressure conditions, and find that they bear an electric charge. We demonstrate that jog density is low and jog pair nucleation mechanism should be considered to model dislocation climb in MgO.

Invited lecture

Invited Lecture

Three stages of work hardening in full atomistic details. Seriously.

Luis Zepeda-Ruiz[1], Alexander Stukowski[2], Tomas Oppelstrup[1], Nathan Barton[3], Rodrigo Freitas[1,4,5], Nicolas Bertin[1], **Vasily Bulatov**[1]

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Over 80 years of dislocation science, many models, theories and even principles have been proposed to describe distinct stages I, II and III observed in straining tests of single crystals. Since early 90's Dislocation Dynamics (DDD) has been heralded as the method to eventually deliver a much-coveted connection between the macroscopic stress-strain response and the underlying dislocation motion. Yet, owing to still remaining problems pertaining to the method's fidelity and computability, we find ourselves perpetually "10 years away" from a glorious day when DDD finally delivers a full stress-strain curve with all the hardening stages fully resolved.

Here we present ultra-large scale Molecular Dynamics simulations of aluminum single crystals subjected to uniaxial tension. We show that appearance (or not) of 3-stage hardening depends on the initial crystallographic orientation of the straining axis and results from crystal rotation. In its turn, crystal rotation is a direct consequence of co-axiality forced on the specimen by the testing machine, the view widely accepted in the phenomenological Crystal Plasticity community since the classical studies of Schmid predating dislocations. Thus, because 3-stage hardening is not an intrinsic property of the material but results from a particular geometric constraint imposed in the standard uniaxial straining tests, it makes little sense to look for any specific physical mechanisms to define and control the notorious transitions from stage I to stage II to stage III. Remarkably, stress-strain behaviors, slip system activity and crystal rotations observed in our high-rate MD simulations are in an exact qualitative agreement with quasistatic experiments suggesting that *physics of crystal plasticity scales*, i.e. dislocation mechanisms defining crystal plasticity response remain the same over 12-1-3 decades of straining rates.

Session 5 – Work Hardening
(Tuesday, September 17, 2019 09:00)

Oral presentation

Plastic relaxation in tantalum single crystals strained far from equilibrium

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Relaxation is a basic yet fundamental behavior observed in a wide range of natural phenomena. In physical systems, relaxation is observed in response to a perturbation in otherwise equilibrium thermodynamic conditions or external fields, e.g. dielectric, magnetic, mechanical, and in numerous other settings. At variance with the common view of relaxation as a process leading the system back to its equilibrium, here we present computational experiments in which model physical systems are driven far from equilibrium and then observed to relax to other driven stationary states that too are far from equilibrium. We base our study of far-from-equilibrium relaxations on recent observations of stationary plastic flow in tantalum crystals subjected to continuous compressive straining. Once the flowing crystal attains a state of stationary flow, the rate is changed abruptly - increased or decreased – and a new state of flow is attained. When relaxation after one such sudden jump in the straining rate is interrupted by another sudden jump in the opposite direction, we observe distinct “memory” effects: the stress first deviates from its ultimate stationary level and only then gradually returns back to it. Similar in appearance to complex relaxations observed in glasses after temperature jumps, here the relaxation is taking place between stationary states of an open system driven far from equilibrium in which mechanical energy of straining is converted into heat via continuous plastic deformation.

Oral presentation

The molecular dynamics study of the mechanisms and kinetics of plasticity in aluminum and copper alloys under high-strain rate

Ilya Bryukhanov
Institute of Mechanics, Lomonosov Moscow State University, Moscow, Russia

The plastic deformation under high-strain rate is studied by molecular dynamic simulation. The rate and mechanism of the nucleation and propagation of partial dislocation loop under high shear stress in aluminum-copper alloys near Guinier-Preston (GP) zones of various diameters are investigated. Dislocation nucleation rates near plain GP Cu-zones have been calculated using mean lifetime method within the range of temperatures between 100 and 700 K. Depending on temperature and applied stress the dislocation can nucleate either from the edge, or from the plain area of a GP zone. The dislocation nucleation is preceded by a generation of defect clusters formed due to local opposite atomic shifts in two adjacent (111) planes by half-length of a Burgers vector of a partial dislocation. The influence of solid solution strengthening on the dynamics of straight dislocations and dislocation loops have been studied in aluminum and copper. The expansion of a partial dislocation loop can be accompanied by the formation of twins *via* a shift of the atoms in the internal region of the loop or the formation of the full dislocation loop.

The model of shear stress relaxation in alloys is constructed using the data from molecular dynamics simulation. It has been found that the process of the formation of new dislocation loops is responsible for the power-law dependence of the shear stress at the top of elastic precursor wave and the initial plastic strain rate observed in shock-wave experiments.

This work is supported by the Russian Science Foundation (RSF), research project №19-71-00080.

Invited lecture

Invited Lecture

Microstructural origin of work hardening in FCC Cu single crystals

Wei Cai[1], Shamseddin Akhondzadeh[1], Ryan Sills[2], Nicolas Bertin[1], Minju Kang[3], Vignesh Kannan[3], K. T. Ramesh[3]
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The efficiency of discrete dislocation dynamics (DDD) simulations has been improved by several orders of magnitude through the development of the subcycling algorithm and its recent GPU implementation on the ParaDiS program. This enabled DDD simulations of single crystal Cu to exhibit a clear strain hardening rate using a single GPU for 2-3 weeks. Such simulations generated a large amount of data from which machine learning tools can be applied to extract physical understandings of the work hardening phenomena. For example, we found that the dislocation network formed under uniaxial [001] loading consists of links whose lengths satisfy an exponential distribution. DDD simulation data for ~100 different loading orientations show that the dislocation link length on each slip system satisfies the exponential distribution (characterized by density ρ and a dimensionless parameter ϕ). These data enabled us to train neural networks to predict the plastic strain rate and multiplicate rate on each slip system, for all loading orientations. A generalized Taylor relation is obtained that accurately predicts the flow stress given ρ and ϕ of every slip system.

We also report the first direct comparison between DDD simulations and experimental stress-strain measurements of bulk single crystals under identical loading conditions. Such a comparison is essential in establishing the fundamental premise of dislocation-based theory of crystal plasticity. The experiments are performed using the desktop Kolsky bar apparatus on single crystal Cu samples, with a nominal strain rate of ~ 10^4 s^{-1}. The actual strain rate is measured as a function of time and applied to the DDD simulation cell. We will present the insights gained from the comparisons between DDD predictions and these experimental observations.

Session 6 – Dislocation Dynamics and Dislocation Climb
(Tuesday, September 17, 2019 11:00)

Oral presentation

Dislocation patterns and the similitude principle: a 3D-DD simulations investigation

Benoit Devincre, Francesca Boioli, Riccardo Gatti
LEM, CNRS-ONERA, CNRS, Chatillon, France

During plastic flow of crystalline solids, dislocation microstructures self-organize in the form of patterns, with a wavelength that is inversely proportional to stress. After decades of investigations, the exact influence of such dislocation patterns with different structures depending on the loading condition, is still under discussion. We show that dislocation patterns verifying the principle of similitude are reproduced from 3D Dislocation Dynamics simulations on a wide range of dislocation density. The simulated patterns are formed in periodic Cu volumes representative of large single crystals deformed in multi-slip. The influences of two specific properties of dislocations, i.e. collinear annihilation and cross-slip, are discussed. This new insight into the collective properties of dislocations has important implications regarding models of crystal plasticity.

Oral presentation

Grain size effects on back stresses induced by GND: A Dislocations Dynamics study

Ghiath Monnet[2], Maoyuan Jiang[2], Benoit Devincre[1]
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During plastic deformation of polycrystal, plastic incompatibility develops at Grain Boundaries (GBs) due to the difference in grain orientation and slip activity. The incompatibility appears at GBs as dislocation walls and dislocation pileups. For dislocation walls, the distribution can be fully described by a singular Nye dislocation density tensor, which is known to induce back stresses inside the deforming grain. While the analytical solutions for infinite walls are known for a long time, the grain size effect on these stresses, specifically the area of the wall, did not receive enough attention in the literature. Dislocation Dynamics (DD) simulations are used to compute stresses as a function of the distance from walls of finite height formed of finite dislocation lines of different characters. It is found that, for all wall configurations, the profiles of the stress components are close to the c^2 – distribution functions: one is monotonously decreasing and one has a maximum close to the grain center. Besides, it is shown that the spatial evolution of the stress components scales invariably with the surface density and the dimensions of the wall. Formula accounting for the dislocation character, wall dimensions and dislocation surface density are established and tested to predict the back stresses prevailing in close grains deforming under different load and boundary conditions. The stress predicted at the grain center in seven different configurations was always found within 20% of stress computed directly in DD simulations.

Oral presentation

Invited Lecture

Dislocation climb and annealing in 3D dislocation dynamics simulations

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Reliable thermal and irradiation creep lifetime prediction is a critical aspect in the design of high-temperature materials used in the aerospace and nuclear components. Critical examples include the mechanical behavior of zircaloy fuel cladding in fission-type water-cooled reactors and the deformation of tungsten in Plasma-Facing Components (PFC) in fusion reactors. These components may experience severe deformation and failure by creep, mediated primarily by dislocation climb and climb-assisted glide. One difficulty with current phenomenological models used in design is that they fall short of predicting creep behavior of irradiated materials outside the data range of the underlying experimental database. This difficulty is exacerbated by the fact that experimental creep tests often provide a limited description of the true long-term response of materials. In order to overcome these limitations, we develop here a predictive model of dislocation climb and annealing at high-temperature and under irradiation. The developed model is based on three-dimensional (3d) Dislocation Dynamics (DD) simulations of climb and glide processes, coupled to a continuum vacancy diffusion boundary value problem (BVP). The unique features of the model are: (1) the solution is available in finite domains to study the effects of grain size on annealing and recovery, and (2) 3d dislocations can undergo simultaneous glide and climb at vastly different time scales. Applications of the model will be shown for BCC tungsten, which is widely considered for PFC applications.

Oral presentation

A new method to investigate dislocation self-climb dominated by core diffusion

Fengxian Liu[1], Edmund Tarleton[1], A.C.F. Cocks[2]
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[2]*Department of Engineering Science, University of Oxford, Oxford, UK*

The mobility of atoms in dislocation core regions is many orders of magnitude faster than in the surrounding lattice. This rapid atomic transport along dislocation cores plays a significant role in the kinetics of many material processes, including low-temperature creep and post-irradiation annealing. In the present work, a finite element based analysis of the dislocation core diffusion process is presented; based on the variational principle. A dislocation self-climb model is then developed by incorporating this finite element core diffusion formulation within the nodal based three-dimensional discrete dislocation dynamics framework. The behaviour of an isolated loop in bcc iron is briefly reviewed, and simulations are extended to include the loop coarsening processes of both parallel and non-parallel loops by self-climb plus glide mechanisms, in which the huge time scale separation between climb and glide is bridged by an adaptive time stepping scheme. Excellent agreements are obtained between the numerical simulation and experimental results, as well as the theoretical solution of rigid prismatic loops. The coarsening process of a population of loops is simulated to investigate the mechanisms of the accumulative interactions and large-scale-patterning in bcc materials.

Invited lecture

Invited Lecture

Advances in dislocation microstructure prediction: A FFT-based Dislocation Dynamics approach

Riccardo Gatti[1], Francesca Boioli[1], Benoit Devincre[1], Lionel Gélébart[2], Laurent Dupuy[2]
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[2]*SRMA, CEA, Saclay, France*

Discrete Dislocation Dynamics (DD) is a well-established simulation technique aimed at reproducing the collective behavior of dislocations at the mesoscale. Despite the considerable progresses made in last decades, DD simulations are still unable to precisely reproduce the microstructure of large poly-crystals and, especially, of irradiated polycrystalline materials. An important step in the development of predictive simulations of this class of materials is the improvement of the numerical capabilities of DD codes to model dislocation properties in large volumes representative of the materials microstructures. Here we propose a promising strategy based on the coupling between two advanced simulation tools. First, the Discrete-Continuous Model (DCM) is employed [O. Jamond et al., Int. J. Plast. 80,19(2016)]. This numerical model based on the Eigenstrain theory, couples an extensive DD simulation code (microMegas), to an elastic solver dedicated to boundary value problems resolution. The DCM allows for the rigorous solution of dislocation-surface and -interfaces interactions and has been proven to efficiently model plasticity in nano- and micro-objects. Nevertheless, its application has been limited to samples of few mm in size. Second, to overcome this limitation, we employ a solver based on Fast Fourier Transform (FFT) calculation. In particular, we employ AMITEX_FFTP, a new distributed parallel elastic solver based on FFT calculation. Using this approach, the stress state definition in the simulated volumes can be computed on very fine grids (e.g. 1024x1024x1024), hence allowing the simulation of realistic dislocation density in a multi-grains periodic volume over significant plastic strains (5-10%). In summary, we aim at improving mechanical properties predictions by taking into account both the complexity of multi-crystalline materials microstructure and the local properties of dislocations.

Oral presentation

Modelling the plasticity of zirconium hydrides

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The presence of hydrides is a major concern for the safety of Zr-alloys for nuclear applications. Hydrides are usually considered as a brittle phase embedded in the ductile metallic matrix. Nevertheless, there is an interesting size effect to be considered. Experimental studies in titanium and zirconium from the literature show that thin micro-hydrides withstand significant plastic deformation without cracking. In both materials slip bands are observed to cross the interface, the critical thickness below which this happens being hundreds of nanometres.

However, the reasons behind this turning point are not understood. In this work, planar discrete dislocation plasticity (DDP) is deployed to investigate this thickness effect. Given the zirconium-hydride orientation relationships, there are two possibilities, as both screw and edge type dislocations are able to cross the interface while satisfying the criteria for slip transmission. Both cases are analysed. Key parameters are the strength of the interface to dislocation crossing and the resistance offered by the hydride to their motion. This controls where dislocations accumulate, and therefore where cracks are likely to be initiated.

It is argued that as the hydride thickness increases, the higher plastic strain to be accommodated causes an increase in the number of internal dislocations. This forest hardening leads to very high internal glide dislocation densities. Furthermore, interfacial dislocations that come from the misfit at the semi-coherent interface may promote the formation of glide dislocation pile-ups in front of the hydride. The two scenarios are explored varying the hydride thickness.

Novel aspects of this study are: the implementation of a screw version of 2D DDP, and its combination with conventional edge 2D DDP to feed into a three-dimensional stress analysis.

Oral presentation

Hydrogen embrittlement defactant concept applied to discrete dislocation dynamics

Jan Inge Meling, Afrooz Barnoush
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Hydrogen Embrittlement is an over 100-year-old problem; its mechanism is unresolved and often contradicting. The Hydrogen Enhanced Localized Plasticity (HELP) mechanism suggests that hydrogen promotes dislocation activity, either by lowering elastic interactions between dislocations or increasing the mobility of dislocations. The Defactant concept, an alternative theory proposed by Kirchheim[1], suggest that hydrogen can lower the energy of defects in the lattice. The reduced defect energy can be applied to nanoindentation results where a lowered pop-in load is reported under the influence of hydrogen[2]. In light of the Defactant concept it can be argued that due to the reduced defect energy of a dislocation loop, homogeneous dislocation nucleation will occur at lower stresses, explaining the Hydrogen effect of lowered pop-ins. In the interest of taking the Defactant concept further, it has been applied within Discrete Dislocation Dynamics (DDD) to investigate the impact of lowered elastic interactions between dislocations. This is done by representing dislocation energy in a simplified manner with the shear modulus, G, and burgers vector, b, as shown in Eq. 1.

Eq. 1: $E_{disl} \sim Gb^2/2$

One can argue that the lowered elastic interaction can be modeled by reducing the burgers vector of dislocations. Simulation results of DDD simulation from 3D Bending models and 2D Crack models will be presented and discussed.

1. **R. Kirchheim, Scr. Mater. 62**, 67 (2010).
2. A. Barnoush, N. Kheradmand, and T. Hajilou, Scr. Mater. **108**, 76 (2015).

Oral presentation

Multi-scale approach of the consequences of hydrogen on cyclic behaviour of nickel single crystal

Guillaume Hachet[1,3], Abdelali Oudriss[1], Afrooz Barnoush[2], Rémy Milet[1], Di Wan[2], Arnaud Metsue[1], Xavier Feaugas[1]
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[3]*CEA - Saclay, Service de Recherches de Métallurgie Physique, Gif-sur-Yvette, France*

A multi-scale study on the influence of hydrogen on cyclically strained oriented nickel single crystal is conducted in order to understand the impact of the solute on the microstructure of strained nickel single crystal. At macroscale, uniaxial cyclic tests are performed to evaluate the impact of pre-charged hydrogen on the work hardening of the material. We noted that hydrogen induces a competition between softening and hardening of the metal. Then, by separating the stress induced by short-range (represented by the effective stress) and long-range (represented by the back stress) interactions between dislocations, we noted hydrogen reduces the effective but has a more complex behaviour with back stress.

Therefore, observations with transmission electron microscope and nano-indentation tests have been performed on cyclically pre-strained nickel single crystal with and without hydrogen. The dislocation organisation induced by the cyclic tests is similar for nickel with and without hydrogen. In both case, the dislocation arrangement can be affiliated to a composite structure with a wall phase containing mainly edge dislocation dipoles and a channel phase where cross-slip event of screw dislocations occurred. We noted that hydrogen impacts the density and the distribution of dislocations and consequently, modifies the internal states of the different phases at microscale. At this length scale, we observed that hydrogen hardens the wall phase while it softens the channel phase. By correlating the results from microscale with the observed competition between hardening and softening effect of the solute at macroscale, we manage to quantify and explain mechanical behaviour of cyclically strained nickel single crystal with hydrogen.

Oral presentation

Deformation mechanisms and twin formation observed in Irradiated ferritic/martensitic steels

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[1]*Laboratory for Nuclear Materials, Paul Scherrer Institut, Villigen, Switzerland*
[2]*Institute of Nuclear Materials, University of Science & Technology Beijing, Beijing, China*
[3]*College of Science, Hunan Agricultural University, Changsha, China*

To study the mechanisms of irradiation-induced embrittlement of ferritic/martensitc steels (FMS), specimens of FMS were irradiated in a target of the Swiss spallation neutron source (SINQ) with high-energy protons and spallation neutrons. The irradiation conditions were in the range of 7.2 – 19.8 dpa (displacement per atom) with 560 - 1750 appm He at 135-300 °C. Transition from ductile fracture of low-dose specimens to brittle fracture of high-dose specimens was observed in tensile tests. After tests, TEM-lamella samples were extracted directly below fracture surfaces using FIB technique. As expected, dislocation channeling phenomenon was observed. Furthermore, for the first time in irradiated FMS, deformation twins were also seen, although just in high-dose and brittle fractured specimens. The twins seem to be initiated at fracture surface, became gradually thinner with distance away from the fracture surface. Features such as twin-precipitates interaction, twin-grain boundary and/or lath-boundary interaction were observed. Twinning bands may be arrested by grain-boundaries or large precipitates, but can penetrate martensitic lath-boundaries. Unlike the case of dislocation channels, small defect-clusters, dislocation loops and dense small helium bubbles were observed inside twin bands. High-resolution TEM observation indicated that the structure of the several atomic layers at twin-boundaries is of fcc structure rather than bcc structure. This implies that the evolution of twining process may be via phase transformation. This hypothesis was confirmed by molecular dynamics (MD) simulation which demonstrated that in iron, at high shear stress levels, transition of bcc structure to fcc structure may take place. Twins are formed when the fcc structure transforms back to bcc. In this contribution, the deformation mechanisms and twin formation in irradiated FMS will be described.

Oral presentation

Invited lecture

Dislocation structure and grain boundary motion induced by nanindentations on STO and W

Karsten Durst, Farhan Javaid
Materials Science, Technische Universität Darmstadt, Darmstadt, Germany

In the present work, the dislocation structure evolution and indentation size effect has been studied for Strontium Titanate (STO) as well as W, using sequential polishing, etch-pits and High-Resolution-Eelectron-Backscattered-Diffraction (HR-EBSD) on pyramidal nanoindentation experiments. STO is used as a model material, allowing a detailed study and a quantification of the dislocation densities at small indentation depth. Nanoindentation load-displacement curves show multiple pop-in events, which relate to nucleation and extension of dislocation pile-ups around the indentations. Sequential polishing and etching revealed the three-dimensional dislocation etch-pit structure at various sub-surface depths. With HR-EBSD, the lattice rotation and thereby GND densities are determined, while the etch-pit technique revealed the total dislocation density. Based on the independently measured dislocation densities, we clearly show a depth dependent dislocation density, where for W and STO the GND densities increase with decreasing indentation depths, leading to the indentation size effect.

Furthermore, the dislocation structure below indentations at the grain boundary (GB) pop-in events were studied for tungsten using electron channeling contrast imaging (ECCI). During indentations in the vicinity of GBs so called GB pop-in events were identified as secondary jumps in the load-displacement curve. A significant hardness increase was observed before the GB pop-in event and the indentation experiments were stopped just after the displacement burst. The careful ECCI analysis on the sequential polished cross-sections clearly shows the dislocation pile-up in the vicinity of the GB along with transmitted dislocations in the adjacent grain. For specific GBs, a GB motion, as evidenced by a GB curvature was observed after dislocation transmission through the GB. The GB motion seems to be coupled with the GB pop-in, indicating a local GB yield process.

Session 8 – Nanoindentation
(Tuesday, September 17, 2019 16:15)

Oral presentation

Plasticity in Au crystals studied by In-situ nano-indentation coupled with bragg coherent diffraction imaging

Stephane Labat[1], Florian Lauraux[1], Thomas Cornelius[1], Marie-Ingrid Richard[1], Oleg Kovalenko[2], Eugen Rabkin[2], Olivier Thomas[1]
[1]*Physics Department, IM2NP - CNRS 7334, Aix Marseille University, Marseille, France*
[2]*Materials Science and Engineering, Technion – Israel Institute of Technology, Haifa, Israel*

The mechanical properties of micro- and nanostructures were demonstrated to vary significantly from their bulk counterparts. Despite numerous studies, plasticity at the nanoscale is, however, not fully understood yet. In-situ experiments are perfectly suited for the fundamental understanding of the onset of dislocation nucleation. Here, we combined in-situ nano-indentation of single-crystalline as well as twinned Au particles with Bragg Coherent Diffraction Imaging (BCDI) that is non-invasive X-ray technique and that is highly sensitive to both strain and defects. Previous BCDI studies on indented Au crystals demonstrated the capability to imaging a single prismatic loop induced by nano-indentation and trapped inside the crystal [1]. Since any movement of diffractometer motors may induce vibrations that eventually lead to damaging the nano-crystal under load, ordinary rocking scans are not suitable for recording 3D reciprocal space maps in-situ. Thanks to the achromacity of the KB mirrors, we scanned the energy of the incident X-ray beam, thus probing the intensity distribution in reciprocal space at different loading steps, thus imaging the evolution of strain and defects (see Fig. 1).

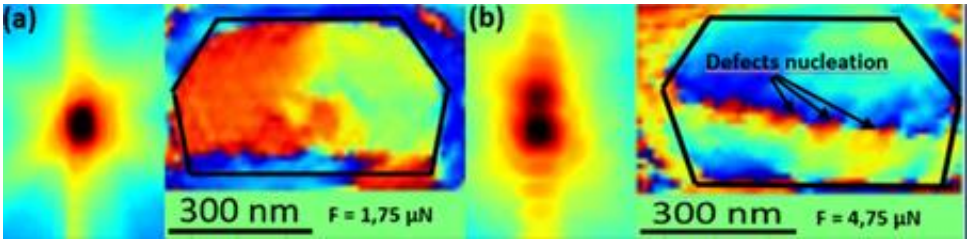

Figure 1: a,b) Qz-Qy integrated images of the core of 3D diffraction patterns for two different mechanical loads and Z-Y cut of reconstructions of the phase for the corresponding mechanical loads.

To the best of our knowledge, this is the first time that E-BCDI has been successfully employed during in-situ experiments providing direct insight into the plasticity at the nanoscale and, in particular, the onset of defect nucleation.

References

[1] - M. Dupraz, G. Beutier, TW. Cornelius, G. Parry, Z. Ren, S. Labat, M.-I. Richard, G.A. Chahine, O. Kovalenko, M. De Boissieu, E. Rabkin, M. Verdier, O. Thomas, Nano Lett. **17**, 6696 (2017)

Invited lecture

Invited Lecture

Dislocation patterning in finite deformation dislocation mechanics and towards plasticity without phenomenological assumptions

Rajat Arora[1], Sabyasachi Chatterjee[1], Giacomo Po[2], Xiaohan Zhang[3], **Amit Acharya**[1], Nasr Ghoniem[2]
[1]*Civil and Environmental Engineering, Carnegie Mellon University, Pittsburgh, USA*
[2]*Mechanical and Aerospace Engineering, University of California, Los Angeles, USA*
[3]*Civil and Environmental Engineering, Carnegie Mellon University, Pittsburgh, USA*

The talk will describe recent progress on two topics: finite deformation dislocation mechanics including patterning and coupling Discrete Dislocation Dynamics to Field Dislocation Mechanics to decribe mesoscale plasticity.

Invited lecture

Invited Lecture

A Phase Field approach to describe the collective properties of dislocations

Istvan Groma
Department of Materials Physics, Eotvos University Budapest, Budapest, Hungary

The plastic properties of crystalline materials are determined by the collective evolution of the dislocation network. A possible approach to follow the complex evolution of a dislocation ensemble is discreet dislocation dynamic simulation but it is a computationally rather demanding task. For many problems another approach is to describe the dislocation network with continuous fields like the statistically stored dislocation density, the geometrically necessary dislocation density, etc. Certainly a key issue here is how to set up the appropriate time evolution equations for the fields introduced. An effective approach applied in several field in physics is the phase field method. It requires a scalar functional of the different fields that is minimized in equilibrium, and appropriate mobility functions determining the dynamics of the system.

For a system of edge dislocations a phase field functional is proposed that is directly derived from the microscopic properties of dislocations. It is show that due to the constrained motion of the dislocations the phase field theory of dislocation density evolution has an unusual character compared to other phase field theories. It is explained how this specific feature leads to dislocation patterning.

In the second half of the talk it is discussed how the phase field approach can be used to couple the evolution of the dislocation system to the evolution of other field like solute atom concentration.

Oral presentation

Large deformation continuum dislocation theory: kinks, jogs and dislocation--vacancy interaction

Thomas Hochrainer, Benedikt Weger
Institute of Strength of Materials, TU Graz, Graz, Austria

It is well-known that plastically deformed crystals contain very high vacancy concentrations. However, crystal plasticity is usually modelled purely conservative. We show that a large deformation theory based on dislocation flux equations naturally leads to jogged dislocation densities which are not tied to a single slip plane. Further dislocation motion will therefore in general not be conservative, such that a co-evolving vacancy concentration field needs to be considered. We therefore conclude that the assumption of conservative crystal plasticity is not tenable in large deformations. Small example calculations are used to illustrate the evolution of kinks, jogs, and vacancy concentrations in continuum simulations of dislocation intersections. Continuum thermodynamics is employed to derive a coupled constitutive theory for dislocation vacancy evolution in large deformations. The resulting theory is discussed in light of recent experimental finding on ductile fracture.

Oral presentation

Strain gradient influence on dislocation dynamics

Paulo Pereira, Sérgio Apolinário
Departamento de Física, Universidade Federal de Pernambuco, Recife, Brazil

Dislocations are topological defects known to be crucial in the onset of plasticity and in many properties of crystals. Classical Elasticity still fails to fully explain their dynamics under extreme conditions of high strain gradients and small scales, which can nowadays be scrutinized. Recently [1], by separating conformal and shape deformations, we constructed a new formalism for two-dimensional (2D) Elasticity and described edge dislocations as finite disclination dipoles. This led us to heuristically obtain that dislocations can be driven by a force that is induced by background density (or hydrostatic strain) gradients. The existence of such mechanism is confirmed through atomistic simulations [1], where we can move and trap individual dislocations using such configurational force. This talk presents an insight about the physical mechanism responsible for this driving force. It also shows how to design atomistic simulations that can quantitatively measure the effects of strain gradients on dislocations.

[1] Pereira, P. C. N. and Apolinario, S. W. S. arXiv:1807.04321 (2018).

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Oral presentation

Invited Lecture

Dislocation network evolution in continuum dislocation dynamics

Katrin Schulz[1], Markus Sudmanns[1], Kolja Zoller[1], Peter Gumbsch[1,2]
[1]*Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany*
[2]*Fraunhofer Institute for Mechanics of Materials, (IWM), Freiburg, Germany*

The dynamics of dislocations as line like objects depends on the applied stress fields and the stress interaction in the dislocation microstructure. However, the evolution of a dislocation system is significantly characterized by the formation of dislocation networks due to dislocation reactions. Modeling dislocation multiplication due to interaction and reactions and the corresponding dislocation network evolution on a mesoscopic scale is an important task for the physically meaningful description of stage II hardening in face-centered cubic crystalline materials. In recent Discrete Dislocation Dynamics simulations it is observed that dislocation multiplication is exclusively the result of mechanisms, which involve dislocation reactions between different slip systems. These findings contradict multiplication models in dislocation based continuum theories, in which density increase is related to plastic slip on the same slip system. An application of these models for the density evolution on individual slip systems results in self-replication of dislocation density.

In this contribution, we introduce a formulation of dislocation multiplication and network evolution in a dislocation based continuum formulation of plasticity. A mechanism-based homogenization of cross-slip and glissile reactions is proposed in three-dimensional facecentered cubic systems. As a key feature, the presented model includes the generation of dislocations based on an interplay of dislocation density on different slip systems. This particularly includes slip systems with vanishing shear stress. The results show, that the proposed dislocation multiplication formulation allows for a physically meaningful microstructural evolution without self-replication of dislocations density. The results are discussed in comparison to discrete dislocation dynamics simulations exposing the coupling of different slip systems as the central characteristic for the increase of dislocation density on active and inactive slip systems.

Invited lecture

Invited Lecture

From experiment to simulation and back – data science approaches for understanding plasticity

Stefan Sandfeld
IMFD/MiMM, TU Freiberg, Freiberg, Germany

Experimental observations and simulation data should – in principle – help to shed light on the „inner workings“ of a physical system, say, a material or specimen. There, the „inner workings“ would be the interaction of microstructural features (such as dislocations) among themselves, with the surfaces of the specimen, or with phase boundaries, to name but a few. Both experiment and simulation, however, suffer from particular problems which in many situations makes it difficult to directly compare them or to use results from one as input or support for the other.

In this presentation, we will start by giving an overview over current attempts for integrating experiment and simulation in the context of dislocation plasticity. We will then demonstrate, on the one hand, how data science approaches might be used to access data from experiments that would be otherwise inaccessible and, on the other hand, how data science also might help to reduce the high level of abstraction inherent to most simulations. With those methods, experiment and simulation might get a little closer to each, thereby helping to understand relevant mechanisms in plasticity and fracture from a new point of view.

Oral presentation

Machine learning a neural network magnesium potential

Markus Stricker[1], Binglun Yin[1], Rasool Ahmad[1], Giulio Imbalzano[2], Michele Ceriotti[2], William Curtin[1]
[1]*Ecole Polytechnique Federale de Lausanne, Laboratory for Multiscale Mechanics Modeling, Lausanne, Vaud, Switzerland*
[2]*Ecole Polytechnique Federale de Lausanne, Laboratory for Computational Science and Modeling, Lausanne, Vaud, Switzerland*

Magnesium is a desirable lightweight structural material but lacks the ductility needed for fabrication and performance. To overcome its limitations, the strongly anisotropic and complex dislocation plasticity in Magnesium and its alloys must be understood. This requires interatomic potentials that capture a wide range of subtle properties including small differences in various dislocation energies. While a very good MEAM-type potential exists for pure Mg, its transferability to alloys has been insufficient to date. Here, we thus first pursue development of a machine learning potential for pure Mg. We use a neural network (NN) framework with the Behler-Parinello symmetry functions to describe atomic environments, with training data obtained from extensive first-principles DFT calculations on metallurgically-relevant properties. We first limit the training data to the same set of data used to fit the MEAM potential and thus study the ability of the NN potential to achieve results comparable to the MEAM potential for equal inputs. We demonstrate broad success of the NN potential, as compared to the MEAM potential. Subsequently we include further data in the training and discuss aspects of the NN potential that might be improvable, and discuss extensions of the general approach to the important Mg-Y alloy.

Oral presentation

Extending the Peierls-Nabarro model using machine learning

Amuthan Arunkumar Ramabathiran
Department of Aerospace Engineering, Indian Institute of Technology Bombay, Mumbai, Maharashtra, India

The Peierls-Nabarro (PN) model is a well known approximation that removes the singularity of the linear elastic stress field of a dislocation by modeling the dislocation core structure as a competition between elastic and surface energies. Despite its many limitations, the PN model provides valuable insight into the dislocation core structure and is significantly more efficient than a full atomistic simulation. A variety of enhancements of the PN model have been proposed in the past to improve upon the various assumptions inherent in the model. In particular, it is standard practice to use atomistically informed models using the gamma surface, introduced originally by Vitek. In this work, we revisit the assumptions involved in using the gamma surface and study non-local extensions of the surface energy on the structure of the dislocation core. We achieve this by constructing a non-local version of the gamma surface, using data from molecular dynamics simulations, by employing both kernel ridge and Gaussian process regression. The resulting enhanced surface energy is used in conjunction with the PN model to study the dislocation core structure. The dynamic changes to the core structure as the dislocation crosses a Peierls barrier are also analyzed using the machine-learned PN model. Comparison with fully atomistic calculations will be provided for special cases involving edge and screw dislocations in metallic and covalently bonded crystalline solids to evaluate the accuracy and efficiency of the proposed extension to the PN model. A comparison of the predictions of the proposed model with other well known regularization techniques to model the dislocation core singularity, and planned future extensions of this work will also be discussed.

Invited lecture

Invited Lecture

Grain Boundary Dynamics = Disconnection Dynamics

David Srolovitz[1,2], Jian Han[2], Kongtao Chen[2], Spencer Thomas[2,3]
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Grain boundary dynamics is controlled by the motion of disconnections - line defects with dislocation/Burgers vector (b) and step character/step height (h). The motion of Disconnection modes (b,h) are determined by bicrystallography. The relative importance of different modes depends on temperatures and driving forces and may be determined from statistical mechanics. In this talk, I will focus on the implication of disconnection dynamics for adsorption of dislocations from the lattice, grain rotation and the overall coupling of microstructure evolution and the mechanics of polycrystalline materials.

Oral presentation

Invited Lecture

Modeling 3-D grain boundary evolution driven by the five-dimensional grain boundary energy landscape

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Grain boundary (GB) evolution plays an extremely important role in the mechanical, thermal and electronic properties of micro/nano-crystalline materials. While there have been numerous efforts focused on the mechanical behavior of stationary GBs, many important properties in materials deformation such as recovery, recrystallization, and grain growth necessitate a dynamic treatment of these internal interfaces. Many of these properties are highly dependent on grain boundary (free) energies, which display complex five-dimensional dependencies on the GB geometry. These dependencies are behind important physical phenomena such as faceting, loss of stability of triple junctions, slip transmission, etc. Here we present a three-dimensional generalization of the Kobayashi-Warren-Carter (KWC) grain boundary evolution model governed by a fully-anisotropic GB energy density that depends on the misorientation and inclination of the grain boundary (Admal et al. [2018]). The model is parameterized using grain boundary energy data from atomistic simulations making it truly predictive. Computing gradient flows of the KWC energy is highly nontrivial due to its singular diffusive nature. Inspired by the thresholding method of Merriman, Bence and Osher (Merriman et al. [1992]), we present a new computational approach for the time evolution of the KWC model that results in a decisive improvement in the computation compared to existing implementations. We show that the evolution of model polycrystals can differ dramatically depending on the type of GB energy functional utilized, with important potential implications on their mechanical response.

References:

Nikhil Chandra Admal, Javier Segurado, and Jaime Marian. A three-dimensional misorientation axis- and inclination-dependent Kobayashi–Warren–Carter grain boundary model. Journal of Mechanics and Physics of Solids, 2018. In review.

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Invited lecture

Invited Lecture

On the role of interface structure, morphology and misfit stresses in dislocation-precipitate interactions

Erik Bitzek, Aviral Vaid, Frédéric Houllé, Hao Lyu
Department of Materials Science and Engineering, Institute I, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

The interactions between dislocations and precipitates can lead to significant strengthening of alloys. Using atomistic simulations, we show that the interaction mechanisms, and subsequently the hardening capacity of precipitates, are critically influenced by the nature of the interface and the misfit stress. In the case of an amorphous interphase boundary (IPB), as for $Mg_{17}Al_{12}$ precipitates in a Mg matrix, dislocations loop around the precipitate and get absorbed into the IPB. Although the situation is reminiscent of Orowan loops left in the matrix, the presence of dislocations in the IPB affects subsequent dislocation-interface interaction in a markedly different manner. The morphology, and in particular the curvature of IPBs, can furthermore drastically influence the misfit dislocation network, as demonstrated using experimentally obtained γ/γ' interface morphologies in Ni-base superalloys. The local IPB orientation not only alters the misfit dislocation core structure, but can also facilitate the formation of ⟨ 100⟩ dislocations. Certain Ni-base superalloys furthermore form γ precipitates inside the cuboidal γ' phase. Our simulations suggest that the misfit stresses caused by the γ precipitates reduce the yield stress of γ' cubes subjected to nanomechanical compression tests. The situation is, however, different when the deformation is not controlled by the nucleation of dislocations. In this case, the γ precipitates lead to an additional hardening that is also observed experimentally. The different contributing factors are analyzed and a new potential strengthening mechanism is described.

Invited lecture

Invited Lecture

In situ TEM and simulation study of shear-migration coupling of grain boundaries

Marc Legros[1,2], Frédéric Mompiou[1,2], Armin Rajabzadeh[1], Romain Gautier[1,2,3], Melvyn Larranaga[1,2], Nicolas Combe[1,2]
[1]*CEMES, CNRS, Toulouse, France*
[2]*Université Paul Sabatier, Université de Toulouse, Toulouse, France*
[3]*Institut P Prime, Université de Poitiers, Poitiers, France*

Nanocrystalline metals (d≤100 nm) possess a much greater resistance to plastic deformation than those with conventional grain size. One of the specificities of these nanocrystals is that they contain a large proportion of grain boundaries (GBs) but virtually no dislocations. Plastic deformation is then thought to occur using alternative paths. Several experiments have shown that in these small-grain materials, the plastic deformation is carried out predominantly by grain boundaries. The dominant mechanism is the so-called shear-migration coupling. Despite a recent increase in simulations studies, its experimental characterization remains very scarce. Aside from experimental obstacles, the problem is very vast as real grain boundaries possess at least 5 degrees of freedom and contains a potentially infinite number of disconnections, a specific defect that combines a step and dislocation character.

We have conducted both in-situ TEM experiments and molecular dynamic simulations using the NEB technique (Nudge Elastic Band). We could show that shear-migration coupling involves and is imposed by the displacement of these disconnections whose origin will be discussed. The question that will finally be addressed here is to whether we should still consider a given GB as a crystalline defect or a network of its own, which mechanical properties (mobility, shear coupling) are governed by its nature or by its defects.

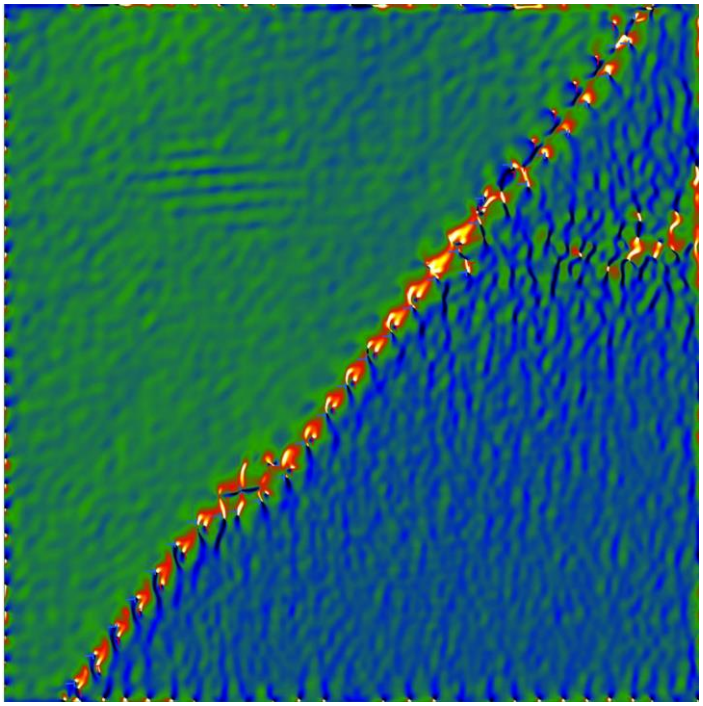

Figure 1: Disconnection observed using a Geometric Phase Analysis of a high resolution TEM micrograph in an Al bicrystal.

Oral presentation

Investigation of the role of disconnections in the shear coupled grain boundary migration mechanism

Melvyn Larranaga, Frederic Mompiou, Nicolas Combe, Marc Legros
CEMES-CNRS, Université Toulouse, Toulouse, France

The grain size reduction in metals (Al, Cu) under less than a few hundreds of nanometers tends to suppress usual intra-granular plasticity, leading to the activation of grain boundary (GB) mechanisms. Among them the shear coupled GB migration has been extensively studied because of its ability to relax strain. It has been shown that this mechanism is the result of the nucleation and propagation of GB defects called disconnections. In order to investigate the role of these disconnections we combine both molecular dynamics (MD) simulations and in-situ transmission electron microscopy (TEM) straining experiments of aluminum bicrystals.

Experimentally, aluminum bicrystal thin foils with Σ3[110](1-1-1) and Σ41[001](540) tilt GB were strained in-situ in the TEM at 400°C in order to favor shear migration coupling. The observations show the propagation of dislocations with a step character along the GB, i.e. disconnections. Moreover lattice dislocations interacting with the GB were frequently observed.

Theoretically, the Σ41[001](540) aluminum bicrystal has been studied using MD simulations. We have first investigated the migration of a perfect GB by calculating the minimum energy path (MEP) using the nudged elastic band method. The configurations along the MEP shows the nucleation and propagation of a pair of opposite disconnections. Because homogeneous nucleation is unlikely to occur in real crystals, we have also investigated the shear coupled migration of the same GB where a simple defect, a row of vacancies, is introduced. We show that the presence of this defect decreases both yield stress at 0 K and energy barriers for the GB migration. We reveal the migration mechanism at the atomic scale of an imperfect GB containing a row of vacancies.

Oral presentation

Kinetic laws for the motion of twin boundaries in ferroic materials: The role of twinning disconnections

Eilon Faran, Doron Shilo
Department of Mechanical Engineering, Technion – Israel Institute of Technology, Haifa, Israel

Twinning is a shear dominated material transition that plays a significant role in metal plasticity, geological processes, and actuation of shape memory and ferroelectric materials. In these materials, twinning transformation proceeds through the motion of twin boundaries as a result of a mechanical / electrical / magnetic driving force. At the atomic scale, the motion of a twin boundary involves the propagation of twinning disconnections, which are interface line defects having both dislocation and step characters. The disconnection`s burgers vector represents the lattice distortion carried by the defect, while the step height determines the amount of transformed volume from one twin to another as the disconnection propagates on the twin boundary.

In this work, we combine direct experimental observations at the level of individual interfaces with analytical modeling, which lead to the extraction and validation of the kinetic relations for twin boundary motion in a ferromagnetic Ni-Mn-Ga crystal. We show that at low velocities, twin boundary follows thermally activated kinetics that are controlled by the nucleation and propagation rates of two dimensional steps whose edges are twinning disconnections. At higher velocities, the twin boundary advances a-thermally as a flat plane. The transition between the two kinetic behaviors takes place at a driving force value that is determined by the magnitude of the lattice barrier for twin boundary motion. Fitting the analytical models to the experimental results allows the extraction of several atomic scale material properties that control twin boundary kinetics. In particular, we evaluate and discuss the magnitude of the line-energy of a twinning disconnection, for both type I and type II twins in Ni-Mn-Ga.

Oral presentation

On interaction of twinning disconnections with obstacles in hcp metals

Andrej Ostapovec
CEITEC-IPM, Institute of Physics of Materials ASCR, Brno, Czech Republic

Mechanical twinning is important mode of plastic deformation in the metals with hcp crystal structure. (e.g. magnesium and titanium alloys). Migration of twin boundaries are often mediated by disconnections. Disconnections are interfacial defects, which combine dislocation and step character. Mechanisms of interaction between disconnections gliding on the {1 0 -1 1} and {1 0 -1 2} twin boundaries and obstacles will be the subject of proposed presentation. Several types of interactions will be considered: interaction with unshearable obstacle, interaction between disconnections and interaction with stacking faults. The nucleation of non-invariant plane facets on the twin boundaries as results of the interaction will be demonstrated as well as disconnection-mediated mechanism of stacking fault growth inside twins.

Invited lecture

Invited Lecture

Understanding dislocation twin boundary interactions: From single twin boundaries towards nanotwinned materials

Christoph Kirchlechner, Maya K. Kini, Nataliya V. Malyar, Juan Li, Gerhard Dehm
Structure and Nano-/Micromechanics, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Nanotwinned materials are known for their enormous strength in combination with an outstanding ductility [1, 2]. Nevertheless, fundamental questions of their deformation behavior are still unanswered today. In the recent past it was proposed that screw dislocation transmit through coherent twin boundaries in copper by a cross-slip-like process. The process also quantitatively fits cross-slip: (i) the stress required for the constriction of two partial dislocations is identical to the transmission stress [3, 4], and (ii), the activation volume of dislocation slip transmission is similar to cross-slip [5]. However, these studies were conducted on a single coherent twin boundary on Cu.

Within this talk we will extend our findings for multiple twin boundaries in Ag. We will present physical vapour deposited Ag thin films with a twin spacing ranging from 20nm to 1µm. Besides the twin-size-scaling we will also discuss statistical aspects of dislocation slip transfer including the role of residual dislocations stored at twin boundaries as well as detwinning. Finally, we will propose a unique dislocation source mechanism at twin boundaries.

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Oral presentation

Atomic simulations of dislocation interactions with coincidence site lattice boundaries in silicon

Simen Nut Hansen Eliassen[1], Jesper Friis[2], Inga Ringdalen[2], Yanjun Li[1]
[1]*Department of Materials Science and Engineering, Norwegian University of Science and Technology, Trondheim, Norway*
[2]*Materials and Chemistry, SINTEF, Trondheim, Norway*

With low production costs and high efficiency, multicrystalline silicon (mc-Si) is widely used in solar cell applications. The crystallization of mc-Si introduces defects which deteriorates the conversion efficiency. Characterization studies suggests that dislocations are positioned at coincidence site lattice (CSL) boundaries. However, such studies are often performed post mortem, thus, the dynamics are not captured. Therefore, an atomistic description of the interactions between the dislocation and CSL boundaries is lacking. To fill in the missing gap, the kinetic Activation-Relaxation Technique (k-ART) has been utilized to simulate the interaction between dislocations and various CSL boundaries. With k-ART, an extensive exploration of the energy landscape is conducted, resulting in full atomistic details of the energy pathways of the interactions, achievable on timescales relevant to experimental studies. In this work, models based on high resolution Transmission Electron Microscope images of the Σ3, Σ9 and Σ27 grain boundaries have been constructed. A pure screw dislocation is placed at various distances from the boundary, and investigated with k-ART. We present here a full picture of the energy landscape for a dislocation to diffuse to the grain boundary and the critical stress required to re-emit the dislocation from the boundary.

Oral presentation

Large scale 3D atomistic simulations of dislocation interactions with bicrystalline interfaces during multiaxial loading

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[3]*Materials Directorate, Air Force Research Laboratory, Wright-Patterson Air Force Base, Ohio, USA*
[4]*NXMM-IMX-STI, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

It is well established that the mechanical properties of polycrystalline materials depend on the interaction between lattice dislocations and grain boundaries (GBs). However, in spite of extensive numerical and experimental studies, the mechanisms behind these interactions are not yet fully understood. To study these complex interaction mechanisms, we recently performed large scale 3D Molecular Dynamics simulations of a screw dislocation interacting with Coherent Twin Boundaries, in a range of face-centered cubic metallic bicrystals modeled with atom method (EAM) potentials. The reaction mechanisms are studied first under uniaxial stress showing that transmission mechanism and critical transmission stress depend on the material considered and differ from results reported in quasi- 2D simulations. Following these first results, we extended this study on two fronts. First, we evaluated the impact of the boundary structure on the interaction mechanism and on the critical stress for transmission, by considering the case of Incoherent Twin Boundaries (ITB) containing ledges. Second, we investigated the influence of multiaxial stresses including shear components in the CTB. We could evidence that the influence of the loading conditions, which can be represented in terms of the Escaig stress is materail dependent. In Al and Cu, the critical transmission stress is largely dependent on the Escaig stress while only mildly for Ni. Additionally, the presence of a shear component in the CTB tends to increase the critical transmission stress for all three materials. The absorption and desorption mechanisms of the screw dislocation are discussed in terms of a potential energy barrier. The simulation results are captured in a mechanistic analytic models aiming to provide input for constitutive equations to be used in mesoscopic simulation schemes.

Oral presentation

The Brittle to Ductile Transition and the core structures of dislocations in silicon

Jacques Rabier
DPMM, Institut Pprime, UPR 3346 CNRS – Université de Poitiers –ENSMA, CNRS, Chasseneuil Futuroscope, France

It is now admitted that perfect shuffle dislocations control the plasticity of silicon in the high stress low temperature domain and dissociated glide dislocations in the high temperature low stress domain. The BDT appears then relevant to the transition between these two domains of "plasticity".

Unlike dissociated glide dislocations, core computations of perfect dislocations show that various core configurations can exist for a given dislocation. Some of these cores are sessile and differently from metals, these sessile dislocations cannot be mobilized under stress promoting the nucleation of crack [2]. TEM experiments have shown that perfect dislocations nucleated in the brittle domain possess very efficient pinning points the density of which increases with temperature [2], [3]. Those pinning points appear to be intrinsic and relevant to some parts of sessile perfect dislocation cores. This induces a shut off of the perfect dislocations sources and a severe discontinuity in the apparent mobility of available dislocations close to the BDT, the consequences of which will be discussed.

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Oral presentation

Kink-limited Orowan strengthening and the brittle to ductile transition of bcc metals

Thomas Swinburne[1], Sergei L. Dudarev[2], Mihai-Cosmin Marinica[3]
[1]*CINaM, CNRS, Marseille, France*
[2]*Theory and Modelling of Materials, Culham Center for Fusion Energy, Oxford, UK*
[3]*SRMP, CEA, Saclay, France*

It is well known that the fracture response of bcc metals and covalent materials undergoes a sharp brittle-to-ductile transition (BDT) with increasing temperature. The classic experiments of Hirsch and Roberts[1] measured the activation energy for the BDT with varying strain rate and provided compelling evidence that the BDT is controlled by dislocation mobility through preexisting microstructure. A critical task for structural nuclear materials science is to gain understanding into irradiation induced embrittlement, which in the Hirsch-Roberts interpretation is manifest as an increase in the BDT temperature due to irradiation defects acting as obstacles to dislocation motion. In this work[2], we use atomistic and mesoscale simulations alongside statistical mechanics to study the motion of kink-limited 1/2 screw dislocations in bcc metals through a field of obstacles, using a recently developed atomistic method[3] to determine the stress and temperture dependent activation free energy of kink pairs in atomistic simulations. Our model predicts the BDT activation energy of unirradiated, unworked bcc metals to be half the kink pair formation energy, a prediction which shows striking quantitative agreement between DFT kink energies and experimentally determined BDT activation energies of Fe, W, Mo and V. With increasing obstacle density under irradiation we predict the BDT temperature to at most double, a relationship we show is satisfied in BDT experiments on low-activation steels.

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Invited lecture

Invited Lecture

On the glide of [100] dislocation and the origin of "pencil glide" in Mg_2SiO_4 olivine: insights from atomic scale modeling

Philippe Carrez, Srinivasan Mahendran, Patrick Cordier
UMET Laboratory CNRS-UMR 8207, University of Lille, Villeneuve d'Ascq, France

Olivine $(Mg,Fe)_2SiO_4$, a silicate with orthorhombic structure, is one of the most common minerals. As an abundant phase of the upper Earth mantle, its plastic properties strongly constrained the thermal convection of Earth mantle in its upper part. Plastic deformation of olivine involves two types of dislocation corresponding to the shortest Burgers vector [001] and [100]. At low temperature and high stress, [001] slip is supposed to be the most predominant slip system whereas at high temperature and low stress, [100] dislocations dominate. Over the last decades, a number of different slip systems have been thus identified in various domain of temperature, strain rate or pressure. In this study, we revisit plasticity of this silicate by computing at the atomic scale the intrinsic properties of dislocation in Mg_2SiO_4 single crystal. All the calculations rely on a parametrized potential combining coulombic interactions and a core-shell interaction model for oxygen atoms. We performed a systematic investigation of [100] dislocations metastable configurations and possible dissociations. Our calculations show that at low pressure, the atomic arrangement within the dislocation core is compatible with the [100](010) slip system observed experimentally. Also we show that the occurrence of several metastable core configurations allows to various cross slip events for which the cross slip energy barrier have been computed. Finally, we will show that the various core configurations and their capabilities to cross-slip give reasonable explanations for the pencil glide mechanism reported experimentally in olivine deformed samples.

Oral presentation

Dislocation mechanisms in TiAl during low cycle fatigue at 800°C investigated by TEM

Soumaya Naanani[1,2], Alain Couret[1], Muriel Hantcherli[1], Catherine Mabru[2],
Jean-Philippe Monchoux[1]
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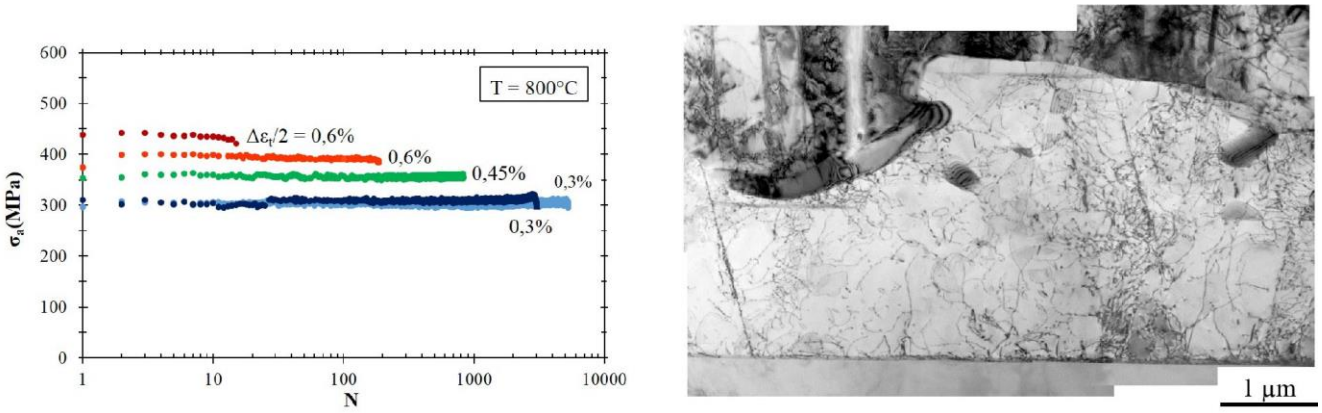
TiAl alloy are promising materials for applications in aeronautical and automotive motors, in reason of their high specific mechanical resistance at high temperatures. However, the behavior of these materials in fatigue, which is an important solicitation mode in service, has principally been explored at the macroscopic scale. Consequently, the elementary dislocation mechanisms remain poorly understood. Here, these mechanisms have been studied for low cycle fatigue (LCF) in traction/compression around 800°C, which are the expected conditions in industrial applications.

The fatigue tests show a remarkably stable behavior (Fig. 1a), without noticeable hardening or softening, a feature which is technologically interesting. Moreover, despite very elevated cumulated plastic deformations (above 500 %), the observed dislocation densities are relatively low (Fig. 1b). Using fine analyses of the dislocation mechanisms by transmission electron microscopy (TEM), these two surprising results are interpreted by a large reversibility of the dislocation motion during the traction and compression steps of the fatigue tests. The probable reason for this reversibility could be the active annihilation by climb of the cross slip loops generated by the numerous forth and back movements of the dislocations, which would thus avoid dislocation multiplication by interactions with the loops. This would then lead to the observed interesting stability of the mechanical properties.



(a) (b)

Fig. 1. (a) Stress amplitude σ_a as a function of cycle number N for various imposed deformations $\Delta\varepsilon_t/2$ in traction/compression LCF at 800°C. (b) Deformation sub-structure after N=5276 cycles, corresponding to a cumulated plastic deformation above 500%. Note the relative low dislocation density considering the large cumulated plastic deformation.

Oral presentation

Systematic investigation of the deformation mechanisms of a γ-TiAl single crystal

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We propose a theoretical framework to predict the deformation mechanism of the γ-TiAl single crystal without lattice defects by combining the generalized stacking fault energy and the Schmid factor. Our theory is validated against an excellent testbed, the single crystal nanowire, by correctly predicting four major deformation mechanisms, namely, ordinary slip, super slip, twinning, and mixed slip/fracture observed during the tensile and compressive tests along 10 different orientations using molecular dynamics simulations. Interestingly, although lattice defects are not taken into account, the theoretical predictions match well with existing experiments on bulk specimen with only a few exceptions; the exceptions are discussed based on the size-dependent deformation mechanism in the presence of preexisting dislocation sources. We expect that the method in this paper can be generalized to study various ductile intermetallic crystals where conventional Schmid law does not hold well.

Invited lecture

Invited Lecture

3D imaging of dislocations with x-rays: recent trends and future prospects

Olivier Thomas[1], Thomas Cornelius[1], Marie-Ingrid Richard[1,2], Stephane Labat[1], Florian Lauraux[1], Jérome Carnis[1,2], Maxime Dupraz[1,2]
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[2]*ESRF, ID01, Grenoble, France*

Dislocations in crystals produce long range rotation and strain fields that allow them to be detected by diffraction. A full quantification of the displacement field is, however, often challenging. The first visualization of dislocations was performed by Hirsch *et al*. [1] in 1956 by transmission electron microscopy (TEM) and TEM has remained since then the tool of choice for imaging dislocations and investigating their dynamics. The very high sensitivity of x-ray diffraction to lattice distortions was early recognized as a strong asset for detecting dislocations in crystals [2]. But, for a long time, the low spatial resolution of x-ray diffraction imaging has limited its large spread use. Strain and defect imaging with x-rays have, however, made very impressive progress lately. On one hand progress in x-ray focusing optics allows nowadays scanning x-ray diffraction mapping to be performed with a resolution in the 50-100 nm range. Full field x-ray microscopy is improving a lot too with resolutions in the 100 nm range [3]. By far the best spatial resolution is obtained with Bragg coherent diffraction imaging (BCDI), which is a lensless imaging technique, with a typical resolution of 6-10 nm [4-6]. BCDI has made impressive progress in the last decade and allows non-destructive 3D imaging of dislocations in various environments (mechanical testing, catalysis, annealing …). I will present and discuss some of these latest results and discuss future prospects opened by new synchrotron sources that are being developed worldwide.

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Oral presentation

Geometrically necessary dislocations in three-point bent Au nanowires studied by in-situ Laue microdiffraction

Thomas Cornelius[1], Zhe Ren[1], Odile Robach[2,3], Jean-Sébastien Micha[2,3],Gunther Richter[4], Olivier Thomas[1]
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In the recent past, the mechanical properties of low-dimensional materials have attracted enormous attention. The yield strength for defect free nanostructures was shown to approach the ultimate limit of the respective material. Despite numerous experimental and theoretical works the mechanical behavior and the onset of plasticity at the nanoscale is still not fully understood. To shed additional light on this topic, *in situ* experimental setups are being designed for monitoring the evolution of the structures during mechanical deformation.

The elastic and plastic deformation of a gold nanowire tested in three-point bending configuration using the custom-built scanning force microscope SFINX was studied *in-situ* by Laue microdiffraction. A new data treatment method, which bases on the integration of diffraction patterns recorded along the deformed nanostructure, was developed visualizing both movement and shape of the diffraction peaks as a function of the measurement position. Besides bending, torsion is evidenced during the elastic deformation originating from a misalignment of the SFINX-tip of the order of 60 nm with respect to the nanowire center. The plastic deformation was found to be governed by the storage of geometrically necessary dislocations. Analyzing the shape of the diffraction peaks, the activation of two unexpected slip systems is found which does not coincide with the slip systems with the highest resolved shear stress. These unexpected slip systems are probably related to the dislocation nucleation process at the clamping point, which is influenced by the local curvature.

Oral presentation

In situ transmission electron microscopy observations of the fcc-hcp phase transformation in Co nanowhiskers

Gunther Richter, Wenting Huang
ZWE Materials, Max Planck Institute for Intelligent Systems, Stuttgart, Germany

Metallic nanowhiskers have shown in the past extraordinary physical properties. In tensile testing experiments, the theoretical strength was reached for various metals. Ferromagnetic materials show single magnetic domain structure. Typical diameters of the nanowhiskers are 100 nm and lengths of up to 50 µm are observed. Therefore these structures are perfect model systems to study materials properties in confined geometries.

In the presentation, we focus on the phase transformation of Co nanowhiskers. Co shows two allotropes, a room temperature hcp crystal structure and above 420°C a stable high temperature phase of hcp structure. For nanoparticles the fcc phase is seen repeatedly. This can be explained by the increasing effect of the lower surface energy for the fcc phase compared to the possible hcp low indexed surface crystal planes.

We investigated the growth of Co nanowhiskers and the onset of the fcc-hcp phase transformation in those nanostructures as a function of temperature as observed in situ a high resolution, high voltage transmission electron microscope. Compared to the perfect crystal structure of fcc nanowhiskers, Co exhibit stacking faults parallel to its axis when observed at room temperature. However, the overall crystal structure is fcc. During thermal cycling partial dislocations are nucleated and propagate parallel to the nanowire axis, forming only a local hcp structure, the overall fcc crystal structure however remains.

Invited lecture

Invited Lecture

The stochastics of strain localization in metallic-glass microwires

Alfonso Ngan[1], Kefu Gan[1], S.S. Jiang[2], H.B.C. Yin[2], Y.J. Huang[2]
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[2]*School of Materials Science and Engineering, Harbin Institute of Technology, Harbin, Heilongjiang, China*

Tensile tests on Cu/Zr-based metallic-glass (MG) micro-wires show observable first yield point, followed by shear fracture on further straining. Microscopy examination reveals discrete shear bands decorating the free surfaces of yielded and fractured MG micro-wires. Both the first-yield and the fracture stress scatter statistically as expected, but surprisingly, they do not exhibit any significant dependence on the wire length.

Fundamentally, while it has been widely accepted that glass plasticity takes place via shear transformation zones (STZs), the knowledge gap between such atomic-sized STZs and the above-mentioned micro/macroscopic plasticity phenomena remains huge. In this work, molecular dynamics (MD) simulations were carried out to delineate the detailed process by which shear bands form from discrete STZs. The results show that the STZs have an increasing tendency to emerge and operate close to one another in a correlated manner along the strain path. This process leads to shear localization in the form of shear bands.

An analytical model is then proposed to relate the probability of the successive operation of discrete STZs, to their nucleation density. The model predicts that, as prior shear events triggers the emergence of new STZs, successive occurrence of discrete shear events speeds up rapidly to an asymptotic state which is exactly the condition of shear localization.

Finally, the MD simulations also indicate that the first observable yield point cannot be due to the emergence and operation of one single STZ. Instead, yield or fracture is controlled by the average or extreme behavior of many STZs or shear bands operated in different locations in the wire, which explains length independence of the MG wire strength – a fact also observed in other glass wires.

Oral presentation

Stochastic behavior of dislocation nucleation from acute and obtuse angles in metallic nanowires

Stav Nisany, Tomer Gur-Apter, **Dan Mordehai**
Department of Mechanical Engineering, Technion – Israel Institute of Technology, Haifa, Israel

Pristine metallic nanowires yield plastically under tensile load by nucleating dislocations from their surfaces. It was commonly accepted that in nanowires with a rhombic cross-section, dislocations are nucleated from edges with acute angles. Using Molecular Dynamics (MD) simulations we show that dislocation nucleation at the onset of plasticity in Pd nanowires can occur from both acute and obtuse angles, with a temperature-dependent probability; nucleation from the obtuse angle is more probable at higher temperature. We quantify this stochastic behavior by calculating the free energy barrier, using MD simulations and the nudged-elastic band method, in combination with the varying driving-force analysis proposed previously for Mo nanoparticles [1]. The free-energy barriers are then incorporated in a Metropolis Monte-Carlo simulation, to predict the nucleation probabilities from each site. Based on the simulation results, we propose a model for the strength distribution of nanowires when nucleation can occur in two site types.

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Oral presentation

Effect of solute atoms and Peierls stress on the critical behaviour of dislocations

Peter Ispanovity[1], Gábor Péterffy[1], Peter M. Derlet[2]
[1]*Department of Materials Physics, Eotvos University, Budapest, Hungary*
[2]*Condensed Matter Theory Group, Paul Scherrer Institut, PSI-Villigen, Switzerland*

It is well-known from micropillar and acoustic emission experiments that in crystalline matter plastic strain accumulates in sudden avalanche-like events. Based on the statistical analysis of these bursts it is now apparent that plastic deformation can be described as a critical phenomenon. Whereas the analysis of experiments suggests that scale-free behavior is characteristic only to the onset of yield, discrete dislocation dynamic (DDD) simulations hint at a more involved picture. Namely, the dynamics of the system is of glassy nature, where power-law distributions arise irrespective of the distance to the yielding threshold [1]. These DDD simulations represent pure systems where neither Peierls stress nor any kind of impurities impede dislocation motion.

In the talk we will discuss how linear stability of the dynamics of the system [2] can be employed to reveal internal dynamic correlations between dislocations in a 2D system. We will show that these correlations are long-range in pure systems and become short-ranged in the presence of point-like impurities or a non-zero Peierls stress. The size and scaling of strain bursts are determined by these correlations: bursts get localized and system size independent in the case of impurities, a fact already observed in experiments. These results, thus, shed light on the microscopic origin of internal length scales affecting the statistical properties of the stochastic plastic response.

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Oral presentation

Nucleation and structure of Van der Waals dislocations in 2D materials

Harley Johnson[1], Shuze Zhu[1], Emil Annevelink[1], Pascal Pochet[2]
[1]*Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA*
[2]*INAC Laboratory for Atomistic Simulation, CEA-Grenoble & Universite Grenoble-Alpes, Grenoble, France*

Two-dimensional materials such as graphene, h-BN, transition metal dichalcogenides like MoS_2, etc., are an emerging class of technologically exiting materials with exotic mechanical and electronic properties. Moiré patterns are commonly observed when these materials are layered, or when they are grown on crystalline metal substrates. To understand these moiré patterns, we introduce the concept of interlayer or van der Waals (vdW) dislocations, and show that arrays of these vdW dislocations constitute the moiré patterns associated with regions of commensurability and incommensurability between the layers. We note that moiré patterns and defects in the moiré patterns themselves are the result of electronic structure signatures of the weak interactions between the layers, locked into place by strong in-plane interactions in the constituent layers. We explain the wide variety of experimentally observed moiré phenomena, including the distinct moiré patterns formed by various combinations of 2D materials on the same metal support layers, as well as point and line defects in moiré patterns. We then present a theory to explain the nucleation of the vdW dislocations in terms of energy reduction in the system. For example, when finite-sized flakes of 2D materials on larger crystalline substrates are made to grow or rotate, vdW dislocations are nucleated; this observation can be understood within the framework of critical thickness theory from classic thin film mechanics. Finally, we explore the connection between vdW dislocations and microstructure formation in 2D materials synthesis, focusing in particular on the distribution of angles and the formation of grain boundaries in polycrystalline 2D material layers.

Oral presentation

Atomistic simulations of stress/strain maps of alloyed nanoparticles

Christine Mottet, Alexis Front
CINaM - CNRS/AMU, CNRS, Marseille, France

In the context of energy, environment and sustainable developments, the prospective replacements for internal combustion engines are proton exchange Polymer Electrolyte Membrane Fuel Cells (PEMFC) where platinum electrodes convert Oxygen and Hydrogen into water via an electrocatalytic reaction. Because of high cost and scarcity of Pt, it is convenient to use Pt-based alloys which can display even better efficiencies than pure Pt catalysts [1]. We propose here a theoretical study of the atomic structure and chemical ordering of Pt-based nanoparticles of alloys (Pt-M, M=Co, Pd, Ag) and in particular the stress/strain map of the nanoparticles since it is well known that the strain has a high impact on the reactivity [2]. We propose a systematic study of the stress/strain map at the atomic scale of nanoparticles of alloys where both the finite size of nanoparticle, the misfit between the two elements and the consequence of phase boundaries or grain boundaries in the core deform the atomic structure at the surface of the nanoparticles where takes place the catalytic reaction. We performed *ab initio* calculations on model and small system , and extensive Monte Carlo simulations on larger ones using semi-empirical many-body potentials to optimize their chemical configurations to get realistic systems to be compared to the experiments [3]. The stress and strain analysis is then obtained by quenched molecular dynamics.

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Nature Communication, accepted (2019)

Oral presentation

Record-breaking strength and solid solution softening in Ni and Ni_3Fe nanoparticles

Amit Sharma[1], James Hickman[2], Oz Mendelsohn[1], Nimrod Gazit[1], Yuri Mishin[2],
Eugen Rabkin[1]
[1]*Department of Materials Science and Engineering, Technion – Israel Institute of Technology, Haifa, Israel*
[2]*Department of Physics and Astronomy, George Mason University, Fairfax, VA, USA*

We demonstrate that faceted single-crystalline Ni nanoparticles produced by solid-state dewetting from a sapphire substrate exhibit an ultrahigh compressive strength (up to 34 GPa) unprecedented for crystalline metals. This strength is consistent with all available estimates of the theoretical strength of Ni. Three factors are responsible for this record-high strength: (1) large shear modulus of Ni (78 GPa), (2) smooth edges and corners of the nanoparticles that reduce the stress concentration during the compression, and (2) thin oxide layer on the particle surface that softens the contacts with the substrate and indenter. This experimental discovery is augmented by molecular dynamics simulations that closely mimic the experimental conditions, including the degree of particle roundness, the softening of the particle contacts with the substrate/indenter, and the testing temperature [1]. We also demonstrate that doping Ni nanoparticles with Fe significantly decreases their strength. This counter-intuitive solid solution softening is attributed to the local misfit stresses around the solute atoms promoting the nucleation of dislocations.

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Oral presentation

Three-dimensional structural imaging of defects in Pt nanocrystals

Marie-Ingrid Richard[1], Jérome Carnis[1], Maxime Dupraz[1], Stephane Labat[1], Lu Gao[2], Jan Philipp Hofmann[2], Nimrod Gazit[3], Eugen Rabkin[3], Emiel Hensen[2], Tobias Schulli[4], Olivier Thomas[1]

[1]*Physics Department, IM2NP-CNRS 7334, Aix Marseille University, Marseille, France*
[2]*Inorganic Materials & Catalysis, Eindhoven University of Technology, Eindhoven, Netherlands*
[3]*Materials Science and Engineering, Technion Israel Institute of Technology, Haifa, Israel*
[4]*Experimental division, The European Synchrotron, Grenoble, France*

At the nanoscale, the properties of materials are largely influenced by elastic strain and depend critically on the presence of crystal defects. However, imaging and characterising the structure of defects inside a crystal in three-dimensions (3D) and *in situ* during reaction remain a challenge. Here, we demonstrate the capabilities of Bragg coherent diffraction imaging [1] to reveal in 3D the structure of defects in Platinum (Pt) nanocrystals and their associated lattice strains. Dislocations are characterised from their characteristic displacement and strain fields (see Figure 1, [2]). We also succeeded to reveal in 3D the detwinning process in a single Pt nanoparticle during *in situ* gas reaction while increasing the O_2 partial pressure [3]. *In situ* and non-invasive structural characterisation of defects during reaction opens new avenues for understanding defect behaviors in confined crystals and paves the way for strain and defect engineering.

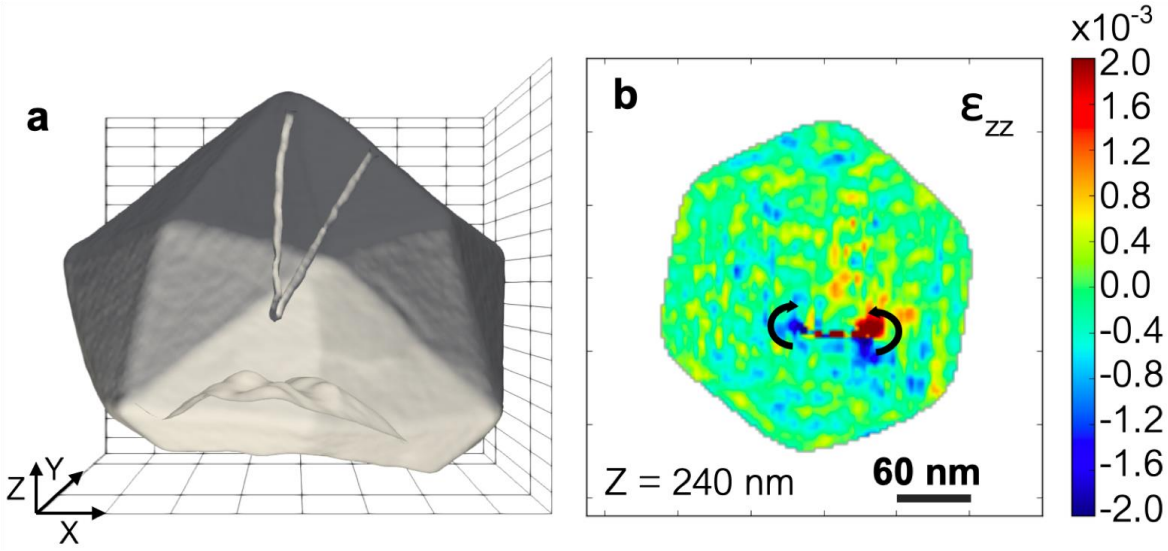

Figure 1: (a) Wireframe plot of the reconstructed electron density of a Pt particle (diameter of 350 nm) drawn at 35% of the maximum density. A dislocation loop is evidenced. (b) Two-dimensional cut of the out-of-plane strain, e_{zz}, at a particle height of 240 nm.

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ABSTRACTS

Poster Presentations

POSTER VIEWING SESSION
(Tuesday, September 17, 2019 20:00)

Poster presentation

A continuum non-singular theory of thermally fluctuating dislocations

Max Boleininger[1], Thomas Swinburne[2], Sergei L. Dudarev[1]
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The simulation of microstructural evolution of materials at temperatures appropriate for fusion operating conditions requires a critical re-examination of fundamental concepts underpinning linear elasticity theory. We find that linear elasticity theory predicts straight dislocations to be unstable with respect to thermal perturbations, which is in striking disagreement with molecular dynamics simulations. Consequently, a dislocation dynamics model based solely on linear elasticity does not provide a sound foundation for the treatment of stochastic thermal fluctuations of dislocation lines.

We propose an atomistically motivated extension of linear elasticity theory that takes into account the physical properties of the edge dislocation core. The resulting model predicts perturbation formation energies qualitatively and quantitatively consistent with predictions derived from molecular dynamics, without need of introducing any empirical parameters. Furthermore, the model offers a first-principles derivation for the commonly used line-tension approximation for the dislocation core energy, and thus represents a fundamental step towards unifying the atomistic and continuum scales in modelling defects and dislocations.

POSTER VIEWING SESSION
(Tuesday, September 17, 2019 20:00)

Poster presentation

Molybdenum plastic deformation: From large scale molecular dynamics simulations towards continuum dislocation dynamics

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Molybdenum (Mo) is an important material for both practical and theoretical purposes. Very high melting of Mo (2896 K) on the one hand make it a promising structural material, on the other hand a wide pressure and temperature range of the BCC phase stability —provides wide simulational opportunities. It is, therefore, a good example for development and calibration of elastic-plastic models.

We perform large scale molecular dynamics simulations of uniaxial compression of Mo along [100] direction. Strain rates 10^7-10^9 /s are considered. Contribution of various hardening mechanism are studied with respect to various strain rates and temperatures to produce a continuum dislocation dynamics (CDD) model. We emphasize that this approach does not require experimental data. The CDD results are in good agreement with various shock-waves experiments.

POSTER VIEWING SESSION
(Tuesday, September 17, 2019 20:00)

Poster presentation

Analysis of austenite-martensite phase boundary and twinned microstructure in shape memory alloys: The role of twinning disconnections

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An austenite-martensite phase boundary in shape memory alloys (SMA) is associated with a periodic microstructure of martensite twin lamellas. Microscopy studies show that the period, which represents the thickness of the twin lamellas, increases with the distance from the habit plane. This observation is often overlooked when the microstructure and energy of the austenite-martensite interface are evaluated. In this paper we introduce a model that reproduces the variation in the twin lamella period. For this purpose, the overall energy of the phase boundary and the accompanied twinned microstructure is formulated and minimized. In particular, the effect of twinning disconnections, via which twins are tapered or broaden, and the additional energy due to the disconnections, are considered. Fittings of model predictions with measurements based on microscopy images provide evaluations of the twin boundary and twinning disconnection energies. Comparison of the results with expressions based on the theory of dislocations indicates that interactions between disconnections play a dominant role in determining the overall energy of twinning disconnections.

POSTER VIEWING SESSION
(Tuesday, September 17, 2019 20:00)

Poster presentation

An effective implicit method for discrete dislocation dynamics simulation

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Dislocations exhibit complex spatiotemporal dynamics due to their long-range mutual interactions via their induced stress fields. The mathematical formulation of this system leads to stiff differential equations. Solving them numerically with explicit methods on long time scales is computationally rather demanding. Nonetheless, all the currently applied algorithms are based on different explicit methods both in 2 and 3 dimensions [1, 2]. Although implicit methods are generally more suitable for such problems, because of the long-range interactions, the computing cost can be even higher for a large number of simulated dislocations or dislocation segments.

To find an optimal intermediate solution we developed an implicit method, which decreases the simulation runtime efficiently in 2 dimensions by reducing the complexity of the mathematical system using physics principles. Our in-depth analysis showed that, while achieving better precision, the runtime decreased with several orders of magnitude. The method can also be applied in 3D systems as well. This numerical scheme is not only significantly faster than previous ones but it also makes it possible to study the precursors of avalanches and the avalanches as well in great depth [3], making it possible to understand better the behavior of dislocation systems during plastic deformation.

1, Papanikolaou, S. and Song, H. and Van der Giessen, E., J Mech Phys Solids 102 (2017)

2, Ryan B Sills and Wei Cai, Model. Simul. Mater. Sci. Eng. 22, 025003 (2014)

3, P. M. Derlet and R. Maaß, Phys. Rev. E 94, 033001 (2016)

POSTER VIEWING SESSION
(Tuesday, September 17, 2019 20:00)

Poster presentation

Observation of diffusion induced dislocations on single Crystalline Au nanowhiskers during interdiffusion studies

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Understanding and control of the defects is a crucial matter in materials science, by analyzing the experimental results, we aim controlled microstructure on nanomaterials, which will open a door for us to optimize the material properties. Therefore, during the interdiffusion studies on bimetallic Au/Fe nanowhiskers we have been coming across so many defect formations and naturally studying them to be able to explain the microstructural changes and diffusion characteristics as well as control and optimize the nanostructures.

Au nanowhiskers were grown on a cold rolled Mo substrate at 750 °C and subsequently a layer of Fe deposited on Au whiskers at room temperature using Molecular Beam Epitaxy (MBE). Au forms random growth of single crystalline nanowhiskers and the layer of Fe shows a mixed crystallinity (Figure 1). After the heat treatments (at 500°C 2h and 600°C 2h), bimetallic nanowire system HRTEM investigations carried out and formation of edge dislocations which later lead to diffusion induced grain boundary formation were observed (Figure 2-3).

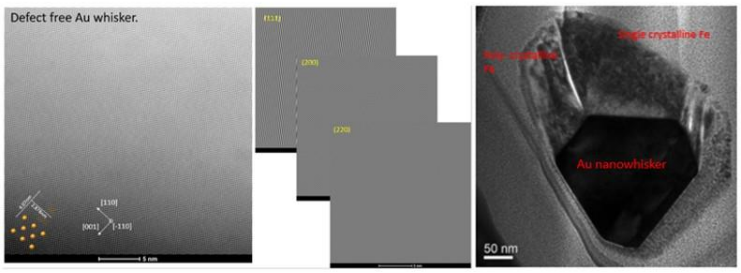

Figure 1. TEM images of the samples before the heat treatments.

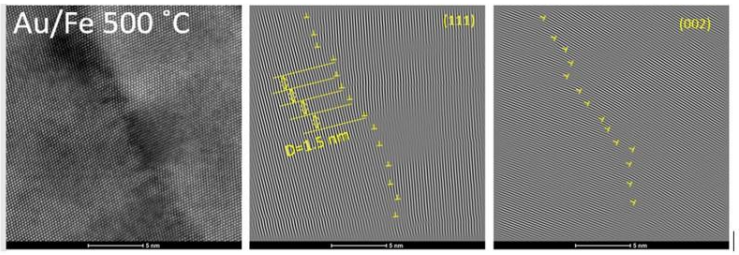

Figure 2. Dislocation formations after 2h at 500 °C.

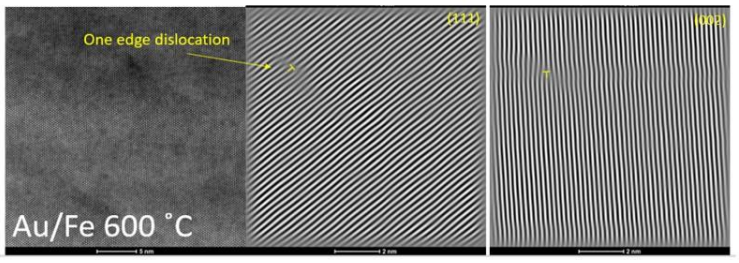

Figure 3. Single dislocation formations after 2h at 600 °C.

POSTER VIEWING SESSION
(Tuesday, September 17, 2019 20:00)

Poster presentation

Critical examination of continuum and cross-core theories of dynamic strain aging

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Dynamic strain aging (DSA) is the process by which solute atoms diffuse towards dislocations and reduce their mobility on the timescale of loading. There are two prevailing DSA theories in the literature: classical continuum theory and cross-core theory. Continuum theory was developed in the early days of dislocation theory, but has been shown to significantly overpredict both the timescale of solute segregation and the resulting strengthening. Cross-core theory was recently developed by Curtin et al. in order to address these shortcomings, and is based on a "single-atomic-hop" diffusive mechanism across the core of an extended dislocation. Whereas these two theories are thought to be distinct from one another in terms of the underlying physics, we show through numerical calculations that in reality there is no major distinction between them. Continuum theory predicts nearly the same behaviors as cross-core theory, as long as the enhanced diffusivity at the core is accounted for; the cross-core solute migration process is not distinct from bulk diffusion. Furthermore, we show that the widely accepted classical expression for solute segregation is incorrect; both the time constant and temporal scaling are in error due to a poor semi-analytical assumption.

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POSTER VIEWING SESSION
(Tuesday, September 17, 2019 20:00)

Poster presentation

Acoustic emission in micropillar deformation experiments

Dávid Ugi[1], Péter Dusán Ispánovity[1], Krisztián Máthis[2], Michal Knapek[2], Istvan Groma[1], Zoltán Dankházi[1]
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Bulk materials generally deform homogeneously. However, if their size is considerably decreased the deformation becomes inhomogeneous and unpredictable. Consequently, traditional methods of metal forming become unusable in this size regime (that is, if the specimen size is around few μm at least in one direction). New probabilistic methods are, therefore, required that take into account the details of random local plastic events. To this end, it is necessary to provide an in-depth experimental investigation of these elementary deformation processes. In my poster, I would like to demonstrate some experimental results, which we achieved by the combination of two experimental methods: (i) nanoindentation testing used to determine the stress-strain characteristics of micrometer size samples, and (ii) acoustic emission measurement which is able to monitor plastic activities in bulk materials. The required micropillars were formed using a focused ion beam from Zn single crystals. The in situ nanoindentation experiment was carried out in a scanning electron microscope while a piezoelectric detector attached to the bottom of the sample recorded the acoustic signals. Our simultaneous measurements show a real correlation between the dislocation avalanches associated with the measured stress drops and the detected acoustic signals. This indicates that the sudden collective motion of dislocations induce the deformation, indeed. We could successfully apply this method to investigate the dependence of the deformation on the size and crystal orientation. Thus we hope that this type of measurement will further deepen our knowledge on the statistical properties of these elementary deformation mechanisms.

POSTER VIEWING SESSION
(Tuesday, September 17, 2019 20:00)

Poster presentation

The Interplay between Dislocation Nucleation and Glide in the origin of the Hugoniot Elastic Limit Spike and Precursor Decay

Roman Kositski, Dan Mordehai
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A common feature in plate impact experiments in annealed body-centered cubic (BCC) metals at room temperature are the “spike and valley” shape of the elastic precursor wave, as well as the decay of the precursor wave called “elastic precursor decay”. In this work, we propose a dislocation-based multiscale continuum strength model that can capture these distinct features. We propose that the origin of these features is in the interplay between dislocation nucleation and dislocation glide. We employ the overstress framework with dislocation glide rules, extracted from atomistic simulations, and we incorporated an Arrhenius-type, stress-dependent, homogenous dislocation nucleation term. Our simulations shed light on the origin of the elastic precursor decay and its fine details. We show that in the early stages of plastic deformation the spike and valley are controlled by dislocation nucleation rather than dislocation glide. As the shock propagates into the specimen, the strain rate decreases, and the relative contribution of dislocation glide to the stress relaxation increases, diminishing the contribution of dislocation nucleation. As a result, the spike and valley vanish and the amplitude of the elastic precursor decays until reaching a steady-state value above a certain propagation distance. The nucleation parameters are calibrated using a metamodel optimization technique using two plate impact experimental results of annealed Ta and V. Using the fitted model we show how the initial microstructure density and temperature affect the elastic precursor evolution, in accordance with experimental results.

POSTER VIEWING SESSION
(Tuesday, September 17, 2019 20:00)

Poster presentation

c+a dislocation glide in zirconium

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Zirconium is a metal with a hexagonal close-packed structure. Plasticity in those metals is usually controlled by glide of dislocations, i.e. dislocations with 1/3 Burgers vector glide. Nevertheless, such dislocations do not accommodate deformation in the direction, for which twinning or glide of c+a dislocation need to be activated. The aim of this work is to understand the c+a dislocation glide based on an both experimental and a numerical approach.

Post-mortem TEM observations on Zr alloys strained to 2% at 350°C have been realized. The glide plane of all observed c+a dislocations is a first order pyramidal plane, in agreement with the literature. Dislocations are aligned in a preferential orientation corresponding to the intersection of the pyramidal plane and the basal plane, thus leading to an almost edge character for these straight dislocations. In situ TEM tensile tests at room temperature have been then performed to understand the glide mechanism of these c+a dislocations.

In order to study the core properties of c+a dislocations, atomic simulations relying on empirical potentials have been used. The potentials have been selected by comparing the obtained stacking faults in all possible glide planes with ab initio results. The core structure of the screw c+a dislocation has then been modeled with two potentials. One potential leads to non-planar dislocation cores dissociated in two different planes, while the other predicts planar cores dissociated in a single plane, with the most stable configuration obtained for a dissociation in a first order pyramidal plane. As TEM observations did not show any lattice frictions for the screw character, non-planar cores appear as an artifact of the empirical potential and the potential leading to a planar dissociation in a first order pyramidal plane is preferred to simulate the glide of c+a dislocations with molecular dynamics.

POSTER VIEWING SESSION
(Tuesday, September 17, 2019 20:00)

Poster presentation

Stress-Dependent activation energy barrier for Cross-Slip in FCC metals

Alon Malka-Markovitz, Dan Mordehai
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Cross-slip is a mechanism by which screw dislocations can change their glide plane and it is an essential mechanism in understanding dislocation-based process and materials modeling. Cross-slip is a thermally activated mechanism and quantifying the stress-dependent activation barrier for cross-slip is crucial. In this work, we present a line-tension model for cross-slip of screw dislocations in face-centered cubic (FCC) metals, with which we calculate the activation energy barrier when Escaig stresses are applied on the primary and cross-slip planes and Schmid stress is applied on the cross-slip plane. A closed-form expression is obtained for the activation energy for cross-slip in a large range of stresses, without any fitting parameters. The model yields results which are in excellent comparison with previous numerical results. By turning one parameter into a fitting parameter, the model results are also in very good agreement with atomistic simulations. Using the closed-form expression, we show that when only Escaig stresses are applied, cross-slip can be energetically unfavorable for a certain relation between these stress. However, Schmid stresses on the cross-slip plane always lower the values of the activation energy and the constraint on cross-slip is removed, i.e., it can occur for all Escaig stresses. This proposed closed-form expression for the activation energy can be easily implemented in dislocation dynamics simulations, owing to its simplicity and universality.

POSTER VIEWING SESSION
(Tuesday, September 17, 2019 20:00)

Poster presentation

Influence of dislocations and Cottrell atmospheres on pressure-induced transformations in single-crystalline iron

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Several studies of pressure-induced phase transformation confirm the appearance of the metastable hexagonal close-packed phase of iron under high pressure. However, the interplay of line and plane defects in the parent material with the transformation process is still not well understood. The principle objective of this project is to understand and explain the role of twins, dislocations and Cottrell atmospheres in changing the crystalline iron structure under high pressure by using classical molecular dynamics simulation. Our results show that the embryos of hcp-Fe are firstly formed at twins under hydrostatic compression. At such conditions, the nucleation of the hcp phase is observed for single crystals containing an edge dislocation. We find that buckling of the dislocation can help to accelerate the transformation process. The crystal orientations between the initial bcc-Fe and hcp-Fe structure are (110)bcc || (0001)hcp. Additionally, the presence of Cottrell Atmospheres surrounding an edge dislocation in bcc iron retarded the development of the hcp phase.

POSTER VIEWING SESSION
(Tuesday, September 17, 2019 20:00)

Poster presentation

A microstructural perspective on the dynamic stored energy of cold work

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Failure of metallic solids under dynamic (impact) loading conditions is a major concern in relation with several extreme engineering situations, such as ballistic impact, vehicle crash or metal forming. Under these conditions, material instabilities - triggered by the short time scales related to dynamic loading - may develop and inevitably precede fracture. During these transient events, and due to the thermo-mechanical coupling effect, part of the supplied mechanical work to plastically deform the material is dissipated as heat. As a consequence, a temperature rise (under near adiabatic conditions) is expected. The remaining, *i.e.*, the non-dissipated work, is stored in the material in the form of microstructural defects (mainly dislocations), which is commonly known as the stored energy of cold work (SECW). The competition between the two, the temperature rise and the SECW, will determine the nature of the material failure. Certainly, the ratio of (adiabatic) thermo-mechanical (plastic work to heat) conversion, commonly known as the Taylor-Quinney factor (TQF), is of great importance when used, *e.g.*, in fully-coupled analysis in numerical simulations.

Dislocations, as the main deformation mechanism present in FCC materials, are used in this work in the form of a continuum and physically-based model to predict the thermomechanical behavior of the material under dynamic conditions, giving an adequate estimation of the stress-strain relation and the TQF. The analytical prediction is compared with the results obtained from an extensive experimental campaign – by means of Kolsky tests and *in situ* infrared measurements - under high rates of deformation.

POSTER VIEWING SESSION
(Tuesday, September 17, 2019 20:00)

Poster presentation

Stable networks containing two pieswise dislocation arrays

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Many observations of networks of piecewise arrays of dislocations are known in many metals after plastic deformation, creep and after annealing. The Frank Bilby equation identifies a small group of low energy networks of two dislocation arrays. The stability of all possible networks comprising of two infinite piecewise arrays of glide dislocations in FCC metals is investigated in the framework of the linear elasticity theory of dislocations. This analysis adds a few additional stable networks to the networks identified by Frank-Bilby equation. These new stable configurations are described and the cause for their stability is discussed.

POSTER VIEWING SESSION
(Tuesday, September 17, 2019 20:00)

Poster presentation

Screw dislocation-carbon interaction in BCC tungsten: An *ab initio* study

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Solutes such as carbon can strongly impact plasticity in BCC tungsten and tungsten alloys. Therefore, we investigated on the interaction between carbon atoms and screw dislocations, which motion controls plasticity of tungsten at low temperature. Since dislocation mobility depends on the defect core region, *ab intio* calculations have been performed to model the dislocation-carbon interaction in tungsten where interatomic bonding is described at the electronic level.

In BCC transition metals, carbon induces a core reconstruction [1] with the dislocations moving from its stable configuration known as the easy core to a hard core configuration which is unstable in the solute-free metal. Our calculations confirm this core reconstruction for large concentration of carbon segregated on the dislocation line in tungsten, corresponding to a strong binding of carbon to the dislocation core. However, this reconstruction is not complete all along the line when the carbon concentration is reduced, contrary to what is obtained in iron-carbon systems [2]. This different behaviour arises from the Peierls potentials of both metals. The hard core configuration' is an energy maximum in the case of tungsten whereas it is a saddle point for iron, thus corresponding to a flat region of the dislocation energy landscape [3]. Finally, calculations have been performed on other interstitial sites in the vicinity of the dislocation, evidencing other possible segregation sites for carbon.

[1] B. Lüthi *et al.*; Modelling and Simulation in Materials Science and Engineering 25; 2017

[2] B. Lüthi *et al.*; Computational Materials Science 148; 2018

[3] L. Dezerald *et al.*; Physical Review B 89; 2014

POSTER VIEWING SESSION
(Tuesday, September 17, 2019 20:00)

Poster presentation

Compression of Nanoporous Au Nanopillars in Molecular Dynamics Simulations

Santhosh Mathesan, Dan Mordehai
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We study the compressive deformation of nanoporous gold nanopillar and the effect of pillar and ligament diameters on the deformation using Molecular Dynamics simulations. Atomistic nanoporous nanopillars are carved from a single crystal FCC lattice with the aid of an algorithm proposed by Soyarslan et al. [1]. The atomic structures are first relaxed, so as to obtain a stable ligament shape and diameter. Then, nanopillars of different diameters with different ligament size are compressed at a constant rate and the stress-strain curves are calculated. The deformation exhibits three typical stages: elastic, a plastic "plateau" and a rapid hardening. Within the elastic regime, we employ a novel technique to identify the average number of load-bearing ligaments, showing that compression of ligaments is predominant. Based on the simulations, we modified the Gibson-Ashby model to account for the size of the nanopillar on the effective elastic constant. In addition, we found that the stress at which the nanopillars yield is size-dependent, explained by the nucleation of dislocations and evolution of stacking faults within the ligaments in the plastic "plateau". Finally, the coalescence of ligaments is observed during the rapid hardening stage. During the densification processes, dislocations are nucleated from the interface until the grain boundary is removed between the two coalesced ligaments.

1. C. Soyarslan, S. Bargmann, M. Pradas, J. Weissmüller, Acta Mater. 149 (2018) 326-340.

POSTER VIEWING SESSION
(Tuesday, September 17, 2019 20:00)

Poster

Compression Strength of Ni-Fe Nanoparticles

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In bulk metals, alloying with another component usually increases the strength of the alloy (solid solution strengthening). However, an experimental work conducted previously in our group showed that alloying the Ni nanoparticles with Fe decreases their strength. This is another indication of the fundamental difference between the plastic deformation of bulk metal samples and of the pristine defect-free metal nanoparticles. For better understanding of the underlying mechanisms of plastic deformation and failure of nanoparticles, we performed Molecular Dynamic (MD) computer simulations that closely mimic the experimental conditions. We have constructed a set of equilibrated particles exhibiting the Wulff shape with rounded edges. The compression of particles of the Ni-25 at %Fe (Ni_3Fe) composition in disordered state, and in the ordered $L1_2$ state was simulated. The compression of the particles of pure nickel was also simulated for the reference. The results of simulations confirm the solid solution weakening observed in the experiment. The obtained results are discussed in terms of the effect of solute atoms on dislocations nucleation.

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