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School of Materials Science and Engineering	
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Brief Introduction

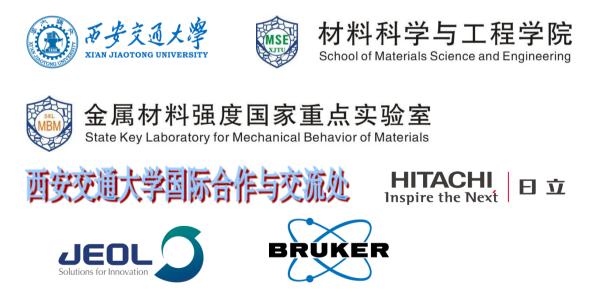
Main Focus

The primary goal of this workshop is to bring together a lineup of well-known scientists, researchers and engineers to review the recent achievements, discuss the current puzzles and share the vision for the future of advancing materials performance from the nanoscale as well as the development of state-of-the-art instruments that enable such explorations, with an emphasis on nanomechanics and *in situ* TEM related topics. The contents include, but not limited to, experimental, theoretical and computational studies of traditional materials, bio materials, energy and battery related materials *et al.*

Program Summary

The workshop will be held at Science Building of Xi'an Jiaotong University from 14 to 16 August. On-site registration is arranged from 2:30 pm to 6:30 pm on August 13 at the lobby of Nanyang Hotel. The breakfast, lunch and dinner on August 14 -16 are included with the workshop registration fee. This workshop will provide a wonderful opportunity to learn the basic knowledge of the proposed topics, communicate with a strong lineup of internationally recognized invited speakers, talk face-to-face with well-established researchers and scientists on their most recent works and be updated on state-of-the-art technologies by leading industry manufacturers.

Sponsors



Map of XJTU Campus





Chairs



<u>Zhiwei Shan</u>

Dean, School of Materials Science and Engineering; Director of Center for Advancing Materials Performance from the Nanoscale (CAMP-Nano), Xi'an Jiaotong University



<u>Ju Li</u>

Professor of Nuclear Science and Engineering and Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge



<u>Evan Ma</u>

Professor of Department of Materials Science and Engineering, Johns Hopkins University, USA



<u>Jun Sun</u>

Director, State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University

Organizing Committee Chair



Weizhong Han

Professor, School of Materials Science and Engineering, Xi'an Jiaotong University Email: <u>wzhanxjtu@mail.xjtu.edu.cn</u>

Invited Speakers

Afrooz Barnoush	Norwegian University of Science and Technology
Christopher Hutchinson	Monash University
Evan Ma	Johns Hopkins University
Gang Sha	Nanjing University of Science and Technology
Gi-Dong Sim	Korea Advanced Institute of Science and Technology
Huiling Duan	Peking University
Jiangwei Wang	Zhejiang University
Jianyu Huang	Yanshan University
Jijun Zhao	Dalian University of Technology
Jose San Juan	University of the Basque Country, Spain
Kai Liu	Tsinghua University
Leyun Wang	Shanghai Jiao Tong University
Marc Legros	CEMES, France
Ming Xu	Huazhong University of Science and Technology
Qihang Liu	Southern University of Science and Technology
Qing Jiang	Jilin University
Qingyu Shi	Tsinghua University
Shigenobu Ogata	Osaka University
Shuai Wang	Southern University of Science and Technology
Upadrasta Ramamurty	Nanyang Technological University

Xianghai An	The University of Sydney
Xiaoyan Zhong	Tsinghua University
Yang Lu	City University of Hong Kong
Yinan Cui	University of California, Los Angeles
Yunzhi Wang	The Ohio State University
Zengguang Cheng	University of Oxford
Zhefeng Zhang	Institute of Metal Research, Chinese Academy of Sciences
Zhenyu Zhang	Dalian University of Technology
Zhuhua Zhang	Nanjing University of Aeronautics and Astronautics

* The list is arranged alphabetically.

August 13th, 2019 (Tuesday)

	14:30 - 18:30	Registration (The Lobby of Nanyang Hotel)
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Time: 8:00 - 11:45, August 14th, 2019 (Wednesday) Location: Room 101, Science Building, XJTU

8:00 - 11:45	Chairs: Upadrasta Ramamurty and Gang Sha	
8:00 - 8:15	Opening Ceremony	
8:15 - 8:45	Evan Ma	Multi-principal-element alloys: a "high-entropy" playground for dislocations
8:45 - 9:15	Gang Sha	Application of APT in understanding high entropy alloys with exceptional properties
9:15 - 10:15	Coffee Break and Group Photo	
10:15 - 10:45	Upadrasta Ramamurty	Additive manufacturing of metals: tailoring microstructures for high mechanical performance and reliability
10:45 - 11:15	Xianghai An	Additively manufactured hierarchical high-entropy alloys with excellent properties
11:15 - 11:45	Jianwei Pan	Recent development in TEM technology of JEOL
12:00		Lunch (Nanyang Hotel)

Time: 14:00 - 21:00, August 14th, 2019 (Wednesday) Location: Room 101, Science Building, XJTU

14:00 - 21:00	Chairs: Leyun Wang and Zhefeng Zhang	
14:00 - 14:30	Zhefeng Zhang	Fatigue strength of Cu-Al alloys with grain sizes from micrometer to nanometer
14:30 - 15:00	Christopher Hutchinson	Dynamic precipitation in aluminum alloys
15:00 - 15:30	Jiangwei Wang	Interface-dominated plasticity in metallic nanostructured materials
15:30 - 16:00	Qingyu Shi	Microstructure and mechanical properties of carbon materials reinforced metal matrix composites fabricated by friction stir processing
16:00 - 16:30	Coffee Break	
16:30 - 17:00	Leyun Wang	Study of the alloying effect on Mg's ductility by in situ synchrotron X-ray and electron microscopy experiments
17:00 - 17:25	Boyu Liu	In-situ TEM investigation on the dislocation behaviors in magnesium
17:25 - 17:45	Jiewen Zhang	Hierarchical 3D nanolayered duplex-Phase Zr with high strength, strain hardening, and ductility
18:00	Dinner (Nanyang Hotel)	
19:00 - 21:00	Po	oster Session (MSE New Building)

Time: 8:00 - 12:00, August 15th, 2019 (Thursday) Location: Room 101, Science Building, XJTU

8:00 - 12:00	Chairs: Jose San Juan and Qing Jiang	
8:00 - 8:30	Qing Jiang	Catalyst design for formic acid dehydrogenation
8:30 - 9:00	Hiroaki Matsumoto	In situ observation of catalyst particles in gas atmosphere using an aberration corrected STEM
9:00 - 9:30	Zhenyu Zhang	Deformation induced new pathways and nanostructures in silicon
9:30 - 10:00	Jijun Zhao	Computational design of novel 2D electronic and magnetic materials
	Coffee Break	
10:00 - 10:30		Coffee Break
10:00 - 10:30 10:30 - 11:00	Jose San Juan	Size-effects on superelasticity ant micro/nano scale in shape memory alloys
	Jose San Juan Yang Lu	Size-effects on superelasticity ant micro/nano
10:30 - 11:00		Size-effects on superelasticity ant micro/nano scale in shape memory alloys Nanomechanics of covalent crystals and their

Time: 14:00 - 18:15, August 15th, 2019 (Thursday) Location: Room 101, Science Building, XJTU

14:00 - 17:50	Chairs: Xiaoyan Zhong and Zhuhua Zhang	
14:00 - 14:30	Zhuhua Zhang	Prediction of synthetic two-dimensional materials
14:30 - 15:00	Ming Xu	Materials gene exploration and modification for 3D phase change memory
15:00 - 15:30	Zengguang Cheng	Chalcogenide phase-change materials for future photonic computing
15:30 - 16:00	Qihang Liu	Rational design principles of quantum anomalous Hall effect from superlattice-like magnetic topological insulators
16:00 - 16:20	Coffee Break	
16:20 - 16:50	Marc Legros	Small-scale plasticity and in situ TEM: intrinsic vs extrinsic approaches
16:50 - 17:20	Xiaoyan Zhong	Atomic scale magnetic and structural imaging by achromatic spatially-resolved electron magnetic circular dichroism
17:20 - 17:50	Eric Hintsala	Correlative microstructural–micromechanical measurements; high Speed, high Vacuum, high temperature
17:50 - 18:15	Jing Hu	Multi scale characterization of corrosion/ hydrogen pick up and in situ ion irradiation of Zr and ATF cladding alloys
18:30	Banquet (Nanyang Hotel)	

Time: 8:00 - 12:00, August 16th, 2019 (Friday) Location: Room 101, Science Building, XJTU

8:00 - 12:00	Chairs: Yunzhi Wang and Huiling Duan	
8:00 - 8:30	Huiling Duan	Mechanical properties of irradiated metallic materials
8:30 - 9:00	Yi-nan Cui	Plastic instability of micrometer-scaled irradiated materials
9:00 - 9:20	Nan Yang	In situ investigation on the behavior of {10-12} deformation twinning in magnesium
9:20 - 9:40	Simian Liu	Effect of ordered helium bubbles on the fracture and deformation behavior of Zr
9:40 - 10:10	Coffee Break	
10:10 - 10:40	Jianyu Huang	In-situ TEM studies of failure mechanisms of lithium ion batteries
10:40 - 11:10	Gidong Sim	Advanced instrumentation and microfabrication for mechanical testing of thin films at elevated temperatures
11:10 - 11:40	Yunzhi Wang	Ordered nanoparticle mediated dislocation transformation in superalloys
11:40 - 12:00	Zhiyu Nie	Controlled growth of aluminum nanowire via thermomigration across a nanoscale junction
12:00		Lunch (Nanyang Hotel)

Time: 14:00 - 17:00, August 16th, 2019 (Friday) Location: Room 101, Science Building, XJTU

14:00 - 17:00	Chairs: Gi-Dong Sim and Yinan Cui	
14:00 - 14:30	Shigenobu Ogata	Atomistic modeling of hydrogen diffusion and hydrogen-enhanced vacancy diffusion in metals
14:30 - 15:00	Afrooz Barnoush	Understanding the hydrogen embrittlement by novel critical experiments
15:00 - 15:30	Shuai Wang	Hydrogen effect on the evolution of microstructure at high strain level
15:30 - 15:55	Junping Du	Hydrogen effect on defect kinetics–A generalized Gibbs isotherm theory
15:55 - 16:20	Dong Wang	Hydrogen embrittlement of high manganese steel examined by small-scale testing
16:20 - 16:40	Longchao Huang	Hydrogen effects on the motion of screw dislocation in α-iron
16:40 -17:00	Closure	
18:00	Dinner (Nanyang Hotel)	

Posters

Wednesday, August 14th, 2019 | 19:00-21:00

Number	Author	Title
Po-001	Sun Kun Choi	Mechanical behavior of metallic thin films passivated by ultra-thin layers
Po-002	Yu Hyun Park	Mechanical characterization of nanotwinned Ni-Mo-W thin films for metal MEMS applications
Po-003	Tingting Jiang	Progressive amorphization of GeSbTe phase-change material under electron beam irradiation
Po-004	Lulu Li	Deformation mechanism of lamellar FeAl/FeAl2 alloy
Po-005	Yujie Jia	Characterization of hydride in zirconium
Po-006	Suyang Sun	Blue phosphorene monolayers as potential nano sensors for volatile organic compounds under point defects
Po-007	Simian Liu	Effect of the ordered helium bubbles on the deformation and fracture behavior of α -Zr
Po-008	Jiangjing Wang	Layer-switching mechanisms in phase change materials
Po-009	Xue Fan	Nanostructure induced mechanical and tribological properties of carbon films studied with in-situ TEM observation
Po-010	Yu Hyun Park	Mechanical characterization of nanotwinned Ni-Mo-W thin films for metal MEMS applications
Po-011	Yongqiang Zhang	Nanogenerator based on the Ohmic-Schottky contact transition in VO2 nanowires

Number	Author	Title
Po-012	Hao Shen	Freeze-casted 3D LLZO porous structure used in composite electrode
Po-013	Jinyong Zhang	Tunable deformation mechanism of strain-transformable Ti alloys with TWIP/TRIP effects
Po-014	Xu Zhang	Effects of twin boundary orientation on plasticity of bicrystalline copper micropillars
Po-015	Jiewen Zhang	Microstructural evolution of nano-layered Zr-2.5Nb during rolling at different temperatures
Po-016	Fei Liu	Novel kink motion of <c+a> dislocations on pyramidal plane in HCP magnesium</c+a>
Po-017	Huanhuan Lu	Visualization of junction growth in metallic single asperity by in situ TEM tribometry
Po-018	Xingyu Feng	The effect of grain boundary structure on intergranular oxidation behavior of 600 Alloy
Po-019	Nanjun Liu	Tunable deformation twins by additional elements in medium entropy alloy CrCoNi
Po-020	Hafiz Muhammad Rizwan Ahamd	Evaluation of band gap and understanding electrical properties of FeS2 by hydrothermal process and first principle study
Po-021	Fan Zhou	Effect of nano-Ti powder additive on microstructure and corrosion resistance of plasma electrolytic oxidation coating on AZ91 Mg alloy
Po-022	Getasew M. Zewdie	Chemical design principles for cache-type Sc–Sb–Te phase-change memory materials

Abstracts

8:15 - 8:45 14th, August

Multi-principal-element Alloys: A "high-entropy" Playground for Dislocations

<u>Evan Ma</u>

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We present systematic atomistic simulations, employing a realistic interatomic potential for the NiCoCr model system, to reveal unusual dislocation behavior in multi-principal-element solid solutions. We demonstrate that these high entropy alloys are indeed different from the familiar (such as FCC) metals and solid solutions, in terms of the ruggedness of the energy landscape that govern dislocation activities. These lead to 10 new features, including 1) low and variable stacking fault energy, 2) local anti-phase boundary energy in the absence of a sublattice, 3) difficulty in nanotwin widening, 4) slip localization resulting in "planar slip", 5) wavy dislocation line, 6) intermittent (stick-slip) nanoscale segment detrapping, 7) small activation volume and higher temperature and strain rate sensitivity, 8) elevated activation energy barrier, 9) elevated lattice friction (mechanical strength), and 10) a playground for tuning properties (in between completely random solution and ordered intermetallics) via ageing at different temperatures. We show how these surprising options confronting dislocations affect the selection of dislocation pathways in slip, faulting, twinning, and martensitic transformation, resulting in behaviors unexpected for conventional FCC metals. We will emphasize as to how the variation in local environments due to concentrated compositions and local chemical order (LCO) necessitates a new mechanism for dislocation motion, strengthening the high entropy alloy. All these open opportunities not accessible to traditional metals and ground-state intermetallics, making HEAs a wonderland for dislocations (and other defects) that control macroscopic properties.

Brief Bio:

The speaker did his graduate work at Tsinghua University and Caltech, followed by postdoc sojourns at MIT and Univ. of Michigan. He is currently a professor in the Department of Materials Science and Engineering at Johns Hopkins University. He has published ~330 papers with ~36,000 citations and h index=100, according to Google Scholar) and presented ~230 invited talks at international conferences and seminars. He has been named a Fellow of ASM International, American Physical Society, and Materials Research Society. Dr. Ma's current research interests include metallic glasses, chalcogenide phase-change alloys for electronics applications, ductility and plasticity mechanisms of nanostructured metals and high-entropy alloys, and TEM of small-volume materials exposed to mechanical, thermal and environmental stimuli.

8:45 - 9:15 14th, August

Application of APT in Understanding High Entropy Alloys with Exceptional Properties

Gang Sha

School of Materials Science and Engineering, Herbert Gleiter Institute of anoscience, Nanjing University of Science and Technology, Nanjing 210094, China

High entropy alloys (multiple main component alloys) exhibit a large composition space and exceptional properties including a good combination of strength and ductility, excellent low temperature performance, irradiation tolerance, unusual catalysis properties etc. These alloys have drawn significant research interests in recent years. The compositions of such alloys have evolved from initially designed equal-components compositions with a single phase to unequal-components compositions with multiple phases in order to get a high strength from multi-phase strengthening such as precipitation-strengthening. In this talks, I will present our jointed research work on understanding several high entropy alloys, including one with a high strength for some special applications, one with attractive low-temperature properties and performance, and one to explore its irradiation defects and the segregation of elements at dislocations in the alloy by using atom probe tomography (APT). The unique information unveiled APT helps to develop better understanding about the complex microstructures of these high entropy alloys.

10:15 - 10:45 14th, August

Additive Manufacturing of Metals: Tailoring Microstructures for High mechanical Performance and Reliability

Upadrasta Ramamurty

School of Mechanical and Aerospace Engineering, Nanyang Technological University, Singapore 639798

Additive manufacturing of metallic components using the selective laser melting (SLM) of powders offers a number of technological advantages and hence, is of considerable current interest for advanced engineering applications. From the scientific perspective, this process offers a number of exciting opportunities, some of which I will discuss in this talk. The SLM process imparts not only a fine microstructure but also distinct mesostructure that depends on the process parameter combinations employed. A complex interplay between these microand meso-structural features can lead to property combinations that were hitherto thought as not possible. In this presentation, some examples as to how all these features will affect the mechanical properties through a comprehensive microstructural and mechanical property characterization of several different alloy components made through SLM will be presented, with particular emphasis on understanding their quasi-static tensile, fracture, fatigue crack growth, and unnotched fatigue properties. Possible avenues for further improvements in properties through post-SLM heat treatments will be discussed.

10:45 - 11:15 14th, August

Additively Manufactured Hierarchical High-entropy Alloys with Excellent Properties

<u>Xianghai An</u>

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High-entropy alloys (HEAs) are a novel class of entropy-stabilized solid solution alloys with five or more principal elements having approximately equiatomic concentrations, which open up a new avenue for the design of materials with optimized properties. The severe lattice distortion and sluggish diffusion that are induced by the mixture of multiple elements endow HEAs with exceptional structure stability and outstanding mechanical properties. However, the current preparations of HEAs rely mainly on the conventional melting or casting methods, imposing enormous limitations to produce samples with complex geometry in terms of cost and efficiency for practical applications. The additive manufacturing (AM) techniques have been recognized as a transformative technology across multiple industries. Based on their advantages of net-shape manufacturing capability and design freedom, it is feasible to harvest parts with complex geometries directly from computer-aided design (CAD) models. In this study, we applied selective laser melting (SLM) technique, which is one of the most popular AM techniques, to prepare near-fully dense HEAs. The as-built samples exhibit a hierarchical nanostructure, including melt pools, columnar grains, dislocations, and sub-micron cellular structures. An outstanding combination of high strength and excellent ductility compared to those fabricated by conventional methods was achieved in the as-built samples. The detailed deformation behaviour, strengthening mechanism and thermal stability will be discussed in this talk.

11:15 - 11:45 14th, August

Recent development in TEM technology of JEOL

<u>Jianwei Pan</u>

14:00 - 14:30 14th, August

Fatigue Strength of Cu-Al Alloys with Grain Sizes from Micrometer to Nanometer

R. Liu^a, Y.Z. Tian^a, Z.J. Zhang^a, P. Zhang^a, X.H. An^{a,c} and Z. F. Zhang^{a*}

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As a significant scientific problem directly impacting on the long-term safety of engineering materials and facilities, the improvement of fatigue strength was comprehensively explored in this study. Advantageous material characters for the improvement of fatigue strength were summarized from the achievements of the previous researches, followed by a new attempt to combine them in material design. As the model material, α -Cu-Al alloys with grain sizes form micrometer to nanometer were thus produced to reveal the effects of grain sizes on the fatigue strength. It is found that the Cu-Al alloys with grain size about 1 µm often display a notable fatigue strength improvement (up to 155 % higher than the coarse-grained counterparts and 40 % higher than the counterparts with nano-scale grain size produced by severe plastic deformation). A general principle briefly summarized as localized fatigue damage reduction was then proposed based on the analysis of the optimizing methods including microstructure optimization and composition optimization. Several recommended features of the high fatigue strength materials were finally listed for further anti-fatigue design, such as uniform grains with small size and stable boundaries; low initial dislocation density, and proper alloying composition.

Keywords: α-Cu-Al alloy; Ultra-fine grain (UFG); Nano-grain (NG); Tensile strength; Fatigue strength.

14:30 - 15:00 14th, August

Dynamic Precipitation in Aluminium Alloys

Christopher Hutchinson

Department of Materials Science and Engineering, Monash University, Melbourne, Australia

High strength Al alloys exploit solid state precipitation to tailor their mechanical response. This precipitation requires two ingredients: a thermodynamic driving force and atomic mobility. For a given alloy chemistry, the heat treatment (precipitation) temperature is chosen as a compromise between having sufficient driving force for precipitation and sufficient atomic mobility so that the precipitation reaction occurs in a reasonable time and results in a 'not too coarse' precipitate distribution. It is this compromise that frames the competition between nucleation, growth and coarsening that constrains the possible precipitate distributions and hence mechanical responses.

In this presentation, we demonstrate a new approach to precipitation hardening that does not use thermal treatments and therefore allows independent control over the thermodynamic driving force and atomic mobility. This provides a means to fully alter the competition between precipitate nucleation, growth and coarsening and new microstructures, with new combinations of properties are obtained.

The approach uses small amplitude cyclic plasticity at room temperature as a means of continually pumping vacancies into the system to achieve atomic mobility and dynamic precipitation under conditions of high thermodynamic driving force. The approach is self-regulating (in both space and particle size) and results in extremely uniform and fine-scale microstructures. The approach can be used either as a new processing route for high strength Al alloys, or as a 'training' routine to improve the high cycle fatigue properties of precipitate strengthened Al alloys. Both examples will be shown in this presentation.

15:00 - 15:30 14th, August

Interface-dominated Plasticity in Metallic Nanostructured Materials

Jiangwei Wang

Zhejiang University

Interfaces, including grain boundaries (GB s), twin boundaries (TBs) and interphase boundaries, critically influence the mechanical properties and deformation mechanisms in metals and alloys. In this talk, we will present our recent progresses on the atomistic mechanisms governing the interface-dominated plasticity in metallic nanostructured materials, using the in situ nanomechanical testing. We revealed that the grain boundaries can migrate reversibly in shear loading cycles through a disconnection-mediated mechanism, in which the nucleation, lateral propagation and dynamic interactions of different types of GB disconnections control the deformation; the dislocation-twin interactions in nanotwinned metallic materials are strongly influenced by the twin size, where the dislocation slip on the uncommon (001) planes can be effectively activated with the twin size decreases; while in metallic nonlamellar materials, the interface structures critically control the deformation, crack formation and fracture. These findings providing novel insights into the interface-dominated plasticity in a broad class of metallic materials.

15:30 - 16:00 14th, August

Microstructure and Mechanical Properties of Carbon Materials Reinforced Metal Matrix Composites Fabricated by Friction Stir Processing

Qingyu Shi *

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Friction stir processing (FSP) is a solid-state processing technology and has unique advantages in fabricating metal matrix composites. During FSP process, the metal matrix will be softened owing to large amount of energy input and a severe plastic flow occurs under the action of the processing tool, resulting in sufficient mixing between reinforcements and metal matrix. In our recent studies, carbon nanotubes (CNTs), graphene (GR) and carbon fibers reinforced aluminum matrix composites are successfully fabricated by FSP. Microstructure observation reveals that the reinforcements are uniformly distributed in metal matrix and clean interfaces are formed between the reinforcements and metal matrix. One interesting thing is noted that most of the reinforcements are distributed in grains. In addition, no visible cracks, metal carbide or impurities are found at the interfaces. The bonding strength of interfaces fabricated by FSP is analyzed by using strengthening models. The results reveal that the reinforcements and metal matrix have strong bonding strength that is close to the shear strength of metal matrix, which is believed to be important for the enhanced mechanical properties. With the addition of carbon materials, the tensile strength, micro-hardness and wear resistant of metal matrix are significantly enhanced. The present findings may provide useful information on fabricating high-performance metal matrix composites reinforced with carbon materials.

16:30 - 17:00 14th, August

Study of the Alloying Effect on Mg's ductility by in Situ Synchrotron X-ray and Electron Microscopy Experiments

Leyun Wang

School of Materials Science and Engineering, Shanghai Jiao Tong University

Room temperature ductility is a bottleneck for the application of Mg alloys as structural material. Recent studies have shown that the addition of yttrium (Y) and calcium (Ca) can potentially improve Mg's ductility. Yet, the underlying mechanism is still unclear. For this presentation, we use both synchrotron X-rays and electron microscopy to understand the issue. In the first work, three dimensional X-ray diffraction (3DXRD) was employed to study slip activity in a rolled Mg-3wt%Y alloy sample that was incrementally loaded by tension. At each load step, 3DXRD data was collected to track the deformation of nearly 1000 grains in the probed volume. By analyzing orientation rotation and stress tensor evolution in those grains, it is possible to identify the activated slip systems and measure their critical resolved shear stress (CRSS) values. The result indicates that Y significantly reduces the CRSS ratio between non-basal <a> slip and basal slip. In the second work, tensile testing of an extruded Mg-0.47 wt.% Ca alloy was conducted inside a scanning electron microscope. EBSD-based slip trace analysis was performed to study in-grain slip activities at different strains. While the majority of the grains were deformed by basal slip, prismatic and pyramidal <a> slip were also frequently observed, and their fractions increased with strain. Schmid factor analysis again indicates a relatively low CRSS ratio between non-basal <a> slip and basal slip in this Mg–Ca alloy. The high ductility in Mg-Y and Mg-Ca alloys are thus attributed to the enhanced activity of non-basal <a> slip.

17:00 - 17:25 14th, August

In-situ TEM Investigation on the Dislocation Behaviors in Magnesium

Boyu Liu, Fei Liu, Zhi-Wei Shan

¹ Xi'an Jiaotong University, Xi'an, P. R. China.

² University of Nevada, Reno, USA.

³ Monash University, Melbourne, Australia.

Magnesium is the lightest structural metal with promising applications for achieving energy efficiency. However, magnesium has limited ductility, which imposes severe constraints on cost-sensitive processing and hampers its widespread applications. The ductility of magnesium is intimately related to the $\langle c+a \rangle$ dislocations. Controversies now abound surrounding the fundamental behavior of $\langle c+a \rangle$ dislocations, such as their ability to accommodate plastic strain and their slip pathways, causing difficulties in rationalizing the mechanical behavior and in alloy design. The present work exploits in-situ TEM mechanical testing and 3D image reconstruction to study the $\langle c+a \rangle$ dislocations in magnesium. The motion of $\langle c+a \rangle$ dislocations of various characters and the slip pathways are investigated. Our experimental strategy can be extended to understanding the dislocation behaviors in other hexagonal metals.

17:25 - 17:45 14th, August

Hierarchical 3D Nanolayered Duplex-Phase Zr with High Strength, Strain Hardening, and Ductility

Jie-Wen Zhang, Wei-Zhong Han*

Center for Advancing Materials Performance from the Nanoscale, State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, P.R. China

Nanolayered, bimetallic composites are highly anisotropic, resulting in limited strain hardening and ductility, due to their 2D planar, unidirectional arrangement. Here we present a novel hierarchical microstructure, comprised of crystals consisting of 3D nanolayered / -Zr networks. By direct comparison with coarse-layered material of the same chemistry, the unusual hierarchical 3D structure gives rise to high strength, strain hardening and ductility. Using TEM analysis and hysteresis testing, we discovered that the 3D randomly oriented biphase boundaries result in progressively dispersive rather than localized slip with increasing strain. Dislocation activity in the α -Zr lamellae transitions from single slip to multislip and eventually to multimodal slip as strain increases. The diffusive slip-promoting properties of 3D layered networks can potentially invoke simultaneous high strength, strain hardening, and ductility, and reveal a new target in the microstructural design of high performance structural materials.

8:00 - 8:30 15th, August

Catalyst Design for Formic Acid Dehydrogenation

Qing Jiang

Key Laboratory of Automobile Materials, Ministry of Education, School of Materials Science and Engineering, Jilin University

Hydrogen economy in automobile industry becomes important especially when China would strive to develop the Hydrogen Fuel Cell Vehicles (FCVs) since 2019. To realize this magnificent target, besides the expensive price of FCVs, suitable hydrogen production and storage techniques must be found. In this report, we introduce the key for the hydrogen production from formic acid, namely the catalyst design where the joint effect of the theory, the simulation, and the experiment has been carried out. The results show that formic acid could take the task as the storage material of hydrogen for FCVs.

8:30 - 9:00 15th, August

In situ Observation of Catalyst Particles in Gas Atmosphere Using an Aberration Corrected STEM

<u>Hiroaki Matsumoto¹,</u> Manabu Shirai¹, Akinari Hanawa¹, Hideki Kikuchi¹ and Hiromi Inada³

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Understanding the evolution of functional materials is highly desired for development and improvement of nanomaterials. For this purpose, *in situ* observation using an environmental transmission electron microscope (ETEM) is one of the most powerful techniques. We have developed a cold field emission (CFE)-ETEM with capabilities of simultaneous SEM with STEM image observation and applied it to the study of Pt/CB electrocatalysts degradation mechanism [1][2]. Recently, target materials are scale down and imaging with sub angstrom resolution is required even *in situ* observation. Recent development of the aberration corrector enable us to observe samples at atomic resolution. Furthermore, micro electro mechanical systems (MEMS) chip-based specimen holders were developed. These holders provide highly stable observation even at high temperature. In this study, *in-situ* observation of catalysis under gas atmosphere using an aberration corrected STEM with a MEMS heating holder is reported.

In-situ observation was performed with an HF5000 200 kV TEM/STEM (Hitachi High-Technologies Co.) equipped with a probe corrector. Figure 1 shows an external view of the HF5000 and a schematic diagram of vacuum system of the HF5000 for environmental (S)TEM imaging. Its standard vacuum system have been modified suitably for *in situ* observation of gas reaction with a differential pumping aperture and an additional turbo molecular pump to improve evacuation system in order to keep the gun pressure low enough to operate CFE. The gas was introduced into the specimen chamber via a gas injection nozzle installed near the specimen chamber. A MEMS-based holder (Blaze, Hitachi High-Technologies Canada, Inc.) was employed for *in-situ* heating observation. Figure 2 shows an external view of the holder. There are electron transparent SiN windows for supporting samples and providing high stability while enabling (S)TEM imaging. Maximum temperature of this holder is 1100 degree Celsius and heating up time from room temperature to 1100 degree takes within a few seconds.

Figure 3 shows ADF-STEM and SEM images of Pt particle on CeO_2 support at 200 degree after O_2 gas injection up to 3 Pa. Atomic columns of Pt particle and CeO_2 support are clearly observed in both STEM and SEM images without specimen drift

and notable scattering effect by gas molecules. It is demonstrated that clear STEM images can be obtained in atomic resolution even at high temperature under gas atmosphere by combined technique with an aberration corrector and a MEMS heating holder. In the presentation, we will report catalytic reaction under various gas atmosphere using the aberration corrected STEM and the MEMS heating holder.

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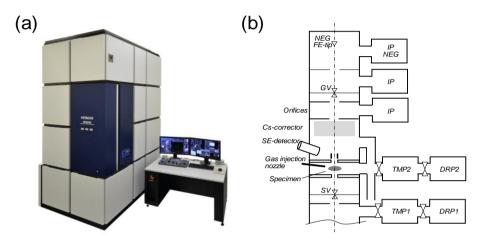


FIG. 1. Overview of HF5000 200 kV TEM/STEM (a) and a schematic diagram of vacuum system of the HF5000 suitable for environmental TEM/STEM (b).

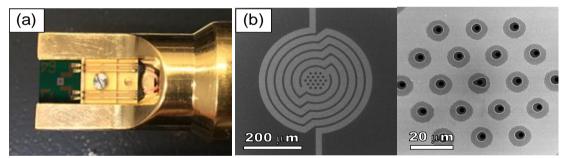


FIG. 2 External view of MEMS heating holder (a) and SEM images of the heating chip (b).

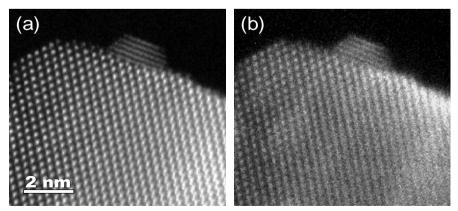


FIG. 3 ADF-STEM image (a) and SEM image (b) of Pt particle on CeO_2 support under O_2 atmosphere at 200 degree.

9:00 - 9:30 15th, August

Deformation Induced New Pathways and Nanostructures in Silicon

Zhenyu Zhang

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Nanostructures in silicon (Si) induced by phase transformations have been investigated during the past 50 years. Nevertheless, the confinement and loading conditions are insufficient to machine and fabricate high performance devices. In this study, grinding or scratching at a speed of 40.2 m/s was performed, on a custom-made setup by an especially designed diamond tip (calculated stress under the diamond tip in the order of 5.11 GPa). A new deformation-induced nanostructure was observed by transmission electron microscopy (TEM), consisting of an amorphous phase, a new tetragonal phase, slip bands, twinning superlattices and a single crystal. A Si wedge is fabricated with a plateau of 80 nm in thickness. In situ dynamic nanoindentation is performed in a transmission electron microscope (TEM) on the damaged Si wedge, using a developed cube corner indenter with a tip radius of 66 nm. A transition from Si-I to Si-VI is demonstrated by in situ atomic characterization, which is a new pathway in Si induced by in situ TEM nanoindentation. The findings propose new insights for fabrication of high performance devices and nanostructure in electronics industry.



9:30 - 10:00 15th, August

Computational Design of Novel 2D Electronic and Magnetic Materials

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Theoretical design based on first-principles computations play an important role in the research and innovation of 2D materials. Very recently, our group has designed a series of novel 2D electronic, magnetic and optoelectronic materials: (1) 2D semiconductor with high carrier mobility including monolayer -Cu2S [1] and eighteen monolayer oxides [2]; (2) Janus group-III chalcogenide monolayers with enhanced piezoelectricity [3]; (3) monolayer group-III monochalcogenides by oxygen functionalization as 2D topological insulators [4]; (2) functionalized SbAs monolayers as spin–valley-coupled Dirac semimetals [5]; (5) monolayer MnB [6], CrSCl and CrSeBr [7] as 2D ferromagnets with high Curie temperature.

Keywords: 2D Materials, carrier mobility; topological insulator, Dirac semimetal, 2D ferromagnets

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10:30 - 11:00 15th, August

Size-effects on Superelasticity ant micro/nano scale in Shape Memory Alloys

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Shape memory alloys (SMA) are functional materials undergoing a reversible martensitic transformation responsible for the shape memory and superelastic effects. In addition, SMA offer the highest work output density, in comparison with other smart materials, and consequently are firm candidates to be incorporated as sensors and actuators into MEMS, because of their ability to undergo a high-displacement actuation during thermal or stress-induced (superelastic) transformation. A good shape memory behavior and superelasticity were reported in Cu-Al-Ni SMA [1-3], and recently a size effect was reported on superelasticity at small scale [4].

The aim of the present work is to overview the stress-induced martensitic transformation, responsible for the superelasticity in SMA, at small scale. First, the experimental methodology, based on nano-indentation techniques, to perform nano-compression tests in pillars milled by focused ion beam with diameters ranging from 2 mm down to 250 nm, will be described. Then, a short review of the state of the art will be offered, before moving to the presentation of the different size-effects observed in SMA at micro/nano scale.

The size-effect on the critical stress for superelasticity in Cu-Al-Ni SMA [4] as well as new results on alternative SMA will be presented. The analysis of the scaling power law for such size effect shows a universal behavior, which will be discussed in terms of the nucleation conditions of the stress-induced martensite. In addition, another size effect on superelastic damping at nano-scale was previously suggested [2], being recently the subject of new long-term studies with view to future applications [5]. The experimental behavior of superelastic damping along thousands of cycles will be described and discussed. Finally an overall analysis of the SMA behavior at small scale will be presented.

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Keywords:Size-effects; Superelasticity; Nano-Compression; Shape Memory Alloys.

11:00 - 11:30 15th, August

Nanomechanics of Covalent Crystals (Silicon and Diamond) and Their Elastic Strain Engineering

<u>Yang Lu</u>

Due to their interesting physical properties, in particular their semiconductor properties, nanoscale covalent crystals such as silicon, germanium and diamond, have stimulated great interests in the past decades. However, to achieve the full potential of these nanoscale building blocks in their electronic and optoelectronic devices will highly depend on their mechanical strength and reliability. In this talk, we show our recent nanomechanical study on one-dimensional (1-D) covalent crystal nanostructures including silicon (Si) nanowires and diamond nanoneedles: Based on our in situ push-to-pull tensile testing, we showed that VLS-grown single crystalline silicon nanowires with diameters ~100nm can be repeatedly stretched above 10% elastic strain at room temperature (Science Advances 2016), with a few cases up to 16% tensile strain, approaching the theoretical elastic limit of silicon; Then we developed a unique in situ push-to-bend method to characterize the bending flexural behavior of nanostructured diamonds, as diamond is the hardest material in nature and usually considered as "indeformable". We found that single-crystalline diamond nanoneedles are capable of undergoing ultralarge elastic bending deformation, up to ~9% local tensile strain (Science 2018), with the corresponding local stress (about 90GPa) approaching the ideal strength of diamond. Beyond mechanics and flexible device applications, such unprecedented large elastic straining, band structures of the nanoscale covalent crystals can be considerably tuned for novel electronics and optoelectronics applications through the "elastic strain engineering".

11:30 - 12:00 15th, August

Elastic Properties and Strain-Induced Buckling of 2-Dimensional Materials

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Interface strain exists very commonly in layered structures, particularly at a hetero-interface of two different materials. Dynamic change of the strain in materials could induce various types of deformations such as bending, rotating, or buckling. In the emerging 2-dimensional (2D) materials, the interface strain exhibits many new features and induces a lot of novel phenomena. In this talk, I will first present the fundamental study of elastic properties of several typical 2D materials, and then summarize the ways to introduce a strain at van der Waals interfaces in 2D materials. It is found that when the strain exists at the 2D material-substrate interface, the geometry of the 2D material can be engineered due to the naturally low interface adhesion. In such a strained system, dynamic web buckling of 2D semiconducting films is in situ observed with a delicately site-controlled initiation. The exploration of these systems not only provides mechanical insight to the understanding of functions and interface physics of layered hetero-structures, but also potentially allows engineering of layered materials as desired.

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14:00 - 14:30 15th, August

Prediction of Synthetic Two-Dimensional Materials

Zhuhua Zhang

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New two-dimensional (2D) materials always bring us surprises with exceptional properties and potential applications. However, synthetic monolayer materials without bulk layered allotropes remain scarce, even if they promise more exotic properties than naturally occurring monolayers through flexible structural options. In this talk, we report a large new family of 2D materials from metal hydrides by high-throughput computational search augmented with first principles calculations. There are 110 thermally and dynamically stable 2D metal hydrides that range from metallic materials to wide-gap semiconductors. A subgroup of these materials even varies topological insulators to nodal-loop semimetals as well as from from antiferromagnetic semiconductors to ferromagnetic half-metals. Unexpectedly, these monolayers resemble graphene in an ability to form weak interlayer interaction due to the variable multicenter bonding of hydrogen. We further report a first-principles design of a tetragonal NbSeH₂ monolayer with substantial magnetism and an indirect band gap of 0.94 eV. Monte Carlo simulations estimate a Curie temperature up to 101 K. Moreover, the monolayer shows high stability and can be extended to a large group of transition metals and chalcogens.

14:30 - 15:00 15th, August

Materials Gene Exploration and Modification for 3D Phase Change Memory

<u>Ming Xu</u>

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Phase-change memory is the most promising candidate for the next generation memory technology. It utilizes the large property contrast between the amorphous and crystalline phases of phase change materials (PCMs), which switches to each other within nanoseconds. In the past decades, a lot of efforts have been devoted to explore how the structure defines the particular properties of PCMs, and it is discovered that the structure of the amorphous phase plays the key role in this case. For example, the fragility of the glass determines the crystallization speed (the programming speed in memory); the glass aging results in the resistance drift in the devices; the stability of the glass (data retention) is determined by the covalent bonds in this material. Since the amorphous phase is absent of long-range order and defects such of as dislocation and grain boundary, the physical properties are usually determined by the short- and medium-range orders, and hence we call it the materials "gene" of glass.

We discovered in the our research that the local structure of PCMs could be described as "octahedral motifs", which can be easily modified by adding different dopants. For example, the carbon, which forms tetrahedral clusters, can increases the stability of the glass to elongate the life of memory devices; the addition of Yi and Sc stabilizes the nuclei in the glass, remarkably accelerating the crystallization speed. The discovery of new PCMs enabled by the Materials Genome Engineering paves the way for the design of high-density 3D phase change memory.

15:00 - 15:30 15th, August

Chalcogenide Phase-change Materials for Future Photonic Computing

Dr. Zengguang Cheng

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Inspired by the great success of fiber optics in ultrafast data transmission, photonic computing is being intensively studied as an alternative to replace or hybridize the electronic computer that is reaching speed and bandwidth limitations. At the same time, the rise of artificial intelligence is driving the quest for non-von Neumann and brain-inspired computing paradigms.

To succeed in mimicking the brain's function from hardware's aspect, two levels have been proposed to implement brain-inspired computing: co-locating storage and processing, as well as artificial neural network. Chalcogenide phase-change materials (PCMs) have been widely used in non-volatile optical and electrical storage due to their superior properties in fast switching speed, high reproducibility and long-term stability. Herein, we combine a typical PCM (Ge₂Sb₂Te₅) with an integrated optical waveguide to build optical devices for the two-level brain-inspired computing aforementioned. First, we develop an optical pulse width modulation (PWM) switching of a PCM unit, which allows for practical co-location of photonic memories and logic functions on a single device. Next, we implement a photonic synapse utilizing a PCM as well with a synaptic plasticity, which is an essential step for photonic artificial neural network.

Keywords: phase-change materials, photonic computing, photonic memory, photonic synapse, artificial neural network

15:30 - 16:00 15th, August

Rational Design Principles of Quantum Anomalous Hall Effect from Superlattice-like Magnetic Topological Insulators

<u>Qihang Liu</u>

As one of paradigmatic phenomena in condensed matter physics, the quantum anomalous Hall effect (QAHE) in stoichiometric Chern insulators has drawn great interest for years. By using model Hamiltonian analysis and first-principle calculations, we establish a topological phase diagram and map on it with different two-dimensional configurations, which is taken from the recently-grown magnetic topological insulators MnBi₄Te₇ and MnBi₆Te₁₀ with superlattice-like stacking patterns. These configurations manifest various topological phases, including quantum spin Hall effect with and without time-reversal symmetry, as well as QAHE. We then provide design principles to trigger QAHE by tuning experimentally accessible knobs, such as slab thickness and magnetization. Our work reveals that superlattice-like magnetic topological insulators with tunable exchange interaction serve as an ideal platform to realize the long-sought QAHE in pristine compounds, paving a new avenue within the area of topological materials.

16:20 - 16:50 15th, August

Small-scale Plasticity and *in Situ* TEM: Intrinsic Vs Extrinsic Approaches

Marc Legros

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Because a wide scientific interest has now focused on materials below the micron scale, in situ Transmission Electron Microscopy (TEM) can be considered as one of the most relevant techniques to investigate possible new processes emerging from confinement effects. The technique already proved extremely useful at unveiling basic deformation mechanisms in micropillars, thin films, nanocrystals and fibers. The development of new sample holders and MEMS platforms, able to perform extrinsic load and displacement measurements inside the TEM could be regarded as the ultimate tool to investigate potential new mechanisms. However, imaging techniques can sometimes provide similar measurements in an intrinsic way (image correlation, dislocation curvature, holography...). Combining both approaches should converge to establish how classical or new mechanisms could explain some of the unexpected small-scale properties of crystalline materials.

16:50 - 17:20 15th, August

Atomic Scale Magnetic and Structural Imaging by Achromatic Spatially-resolved Electron Magnetic Circular Dichroism

Xiaoyan Zhong

National Center for Electron Microscopy in Beijing, Key Laboratory of Advanced Materials (MOE), The State Key Laboratory of New Ceramics and Fine Processing, School of Materials Science and Engineering, Tsinghua University, Beijing 100084, P.R. China

The atomic-level knowledge of local spin configuration of the magnetic materials is of great importance to predict and control their physical properties, in order to meet the challenges of ever-increasing demands on performance of functional materials. However, it is highly challenging to experimentally characterize magnetic properties of such materials with atomic scale spatial resolution. In principle EMCD [1] can offer higher spatial resolution and greater depth sensitivity due to the short de Broglie wavelength and penetration of high-energy electrons compared to XMCD. Recently by using EMCD and achromatic electron microscopy, we are able to access the magnetic circular dichroism with atomic plane resolution [2]. Combining with advanced capability of structural and chemical imaging by using aberration-corrected transmission electron microscopy, all the information including magnetic polarization, atomic configurations and chemical states can be simultaneously accessed from the very same sample region. In the examples of complex oxides e.g. Sr_2FeMoO_6 [2] we would like to show how to achieve local atomic-scale magnetic, chemical and structural information and understand the structure-property relationship of these magnetic materials at the atomic level.

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17:20 - 17:50 15th, August

Correlative Microstructural–micromechanical Measurements; High Speed, High Vacuum, High temperature

<u>Eric Hintsala</u>¹, Youxing Chen², Douglas Stauffer¹, Stuart Malloy³, Nathan Mara⁴

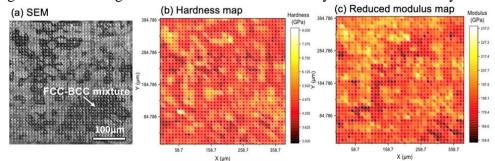
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³ Los Alamos National Laboratory

⁴ University of Minnesota

Materials development for next-generation alloys in critical applications, such as a nuclear reactor, requires high-throughput methodologies. This is due to the number of alloy permutations, processing routes, and operando conditions to be evaluated. One technique that provides highly localized mechanical data is nanoindentation, which can provide statistical datasets at length scales that allow not just macro behavior, but behavior at microstructural length scales to be evaluated.

Here, a new nanomechanical test system, capable of elevated temperature testing under vacuum, enables mechanical mapping under reactor-based conditions typically off-limits to nanoscale mechanical measurements due to oxidation, thermal drift, or their combination. This system provides mapping capabilities at indent per second rates that reduce the effects of tip-sample reactions, thermal drift, and time to test. Therefore, large maps can be acquired at temperatures of interest. These high temperature maps are then correlated to other microstructural techniques, such as EBSD and HR-TEM on several high entropy alloys. These HEAs belong to the same family, based on Al_x FeCrNiMn with varying Al concentration. Three distinct microstructures are presented. Key findings include that except for a bcc-precipitate/fcc matrix material, high strength is maintained up to 400 °C, and measurable mechanical contrast between phases is obvious in all tests. Machine learning based clustering algorithms are utilized to assign phases to each data point in the mechanical maps to get phase specific statistics, speeding analysis drastically.

High throughput mechanical mapping is a means of screening materials for extreme environments, with the ability to generate large statistical datasets with small sample sizes and limited time. Two of the three alloys tested can now proceed to irradiation testing thanks to their good thermo-mechanical stability as characterized by this study.



CAMP-Nano, Xi'an, China, August 14-16, 2019

Figure 1: (a) SEM micrograph of region of dual phase high entropy alloy after nanoindentation mapping at room temperature and (b,c) the resulting hardness and reduced modulus map.

8:00 - 8:30 16th, August

Mechanical Properties of Irradiated Metallic Materials

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The response of metallic materials under extreme conditions is a major concern for engineering applications. For example, the experimentally detectable defects and helium (He) bubbles are formed in metallic materials through displacement cascade and nuclear transmutation reactions during the high energy neutron irradiation process. These irradiation-induced defects and He bubbles can dramatically affect the macroscopic mechanical behavior of metallic materials. In this work, a multi-scale model is proposed to predict the mechanical properties of polycrystals under extreme conditions, which ranges from micro-scale (dislocation level), meso-scale (grain level) to macro-scale (polycrystalline level). At the dislocation level, the evolution law of microstructures (e.g. defects, interfaces and forest dislocations) affected by temperature is characterized through the dislocation-microstructure interaction. At the grain level, the temperature dependent hardening behavior is evaluated by considering their influences on the critical shear resistance to dislocation movement. At the polycrystalline level, elastic-visco-plastic self-consistent method and crystal plasticity finite element method are applied for the scale transition from individual grains to the macroscopic polycrystal, taking into account not only the crystal orientation distribution but also the interaction between adjacent grains. The proposed model can predict the effects of irradiation-induced defects and temperature on the mechanical properties of metals, including irradiation hardening and irradiation embrittlement under high temperature. For ion-irradiated metallic materials, an indentation size effect model incorporating the elastic deformation is developed for modelling the depth-dependent hardness, which takes into account the indentation size effect, ion irradiation induced damage gradient effect and unirradiated region acting as a soft substrate.

8:30 - 9:00 16th, August

Plastic Instability of Micrometer-scaled Irradiated Materials

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Plastic instability is a significant concern in fundamental science and a wide variety of applications, including geophysical solid deformation, machinability, and the design of reliable materials. In particular, plastic instability is widely observed in irradiated materials, and is one of the most important catastrophic failure origins, and thus must be understood at a fundamental level. However, and until now, a clear quantitative understanding of what determines the plastic instability in irradiated material remain as challenging questions. The main difficulty resides in the paucity of systematic experiments under controlled conditions and the significant computational difficulties because of the high density of nanoscale irradiation defects. To overcome this difficulty, we developed a hybrid continuum-discrete model for the collective dynamics of dislocations in dense irradiation defect field [1,2]. New results on the microscopic behavior of dislocations in irradiated materials are revealed, by analyzing the spatial and temporal characteristics associated with plastic deformation as a result of the dynamics of collective dislocation motion in irradiated materials [3,4]. We show the scaling laws for dislocation avalanches and how they lead to the emergence of organized dislocation structures in dislocation channels. Spatial correlation characterization methods are developed and used to obtain information on the width of shear bands resulting from spatial instabilities. The effects of radiation-induced barriers to dislocation motion and the influence of sample size on temporal and spatial plastic instabilities are discussed. A simplified branching model of dislocation source activation is extended to predict dislocation barrier effects on strain burst statistics [5,6]. This finding has implications to the design of radiation-resistant materials.

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9:00 - 9:20 16th, August

In situ TEM Investigation on the Behavior of {1012} Deformation Twinning in Magnesium

Nan Yang, Boyu Liu, Zhiwei Shan

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{1012} deformation twinning plays an important role in the plastic deformation of magnesium. The morphology {1012} twin boundary (TB) is sometimes irregular, and can change during TB migration. This is attributed to the coexistence of {1012} coherent TBs (CTBs) and basal-prismatic interfaces (BPs). However, there is less understanding on the influence of strain condition on the change of TB morphology. In the present work, by performing in situ non-uniaxial compression tests on submicron magnesium pillars, we observed that a {1012} TB can transit into its conjugated TB, (1012) TB to (1012) TB, when the shear strain produced by the initial twin variant cannot accommodate the external applied strain induced by the indenter. We proposed that such transition arise from the interconversion CTBs and BPs to adapt the complex deformation condition.

9:20 - 9:40 16th, August

Effect of Ordered Helium Bubbles on Deformation and Fracture Behavior of α-Zr

Si-Mian Liu¹, Shi-Hao Li¹, Wei-Zhong Han^{1,*}

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Radiation-induced helium bubbles are detrimental to the mechanical properties of metals, usually causing severe hardening and embrittlement. Hexagonal close-packed (HCP) α -Zr alloys are one of the primary structural materials for nuclear applications, however, the effect of helium bubbles on their deformation and fracture behaviors still remains unexplored. Here, we found that ordered helium bubbles prefer to align along the basal plane in HCP α -Zr. Micro-scale in situ tensile tests revealed that helium bubbles less than 8 nm in size can increase the critical resolved shear stress of the prismatic slip. However, once the helium bubbles are larger than 8 nm, a bubble-softening effect appears due to a decrease in number density of helium bubbles and an increase in porosity. Once the Schmid factor of basal slip is considerably higher than prismatic slip, bubble coalescence along the basal plane becomes the major failure mode in helium-irradiated α -Zr.

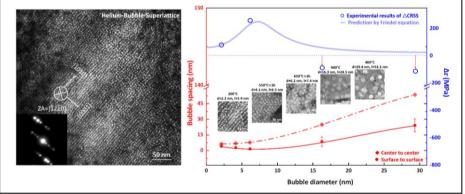


Figure 1. The ordered helium bubbles and the variation of bubble spacing and $\Delta \tau$ for the prismatic slip versus the bubble diameters.

10:10 - 10:40 16th, August

In-situ TEM Studies of Failure Mechanisms of Lithium Ion Batteries

<u>Jianyu Huang</u>

10:40 - 11:10 16th, August

Advanced Instrumentation and Microfabrication for Mechanical Testing of Thin Films at Elevated Temperatures

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Thin films are widely used as functional and structural elements in micro-electronic devices. Therefore, understanding the mechanical behavior of thin films at different length scales and environmental conditions is essential for the design of reliable devices. However, it is difficult to precisely measure the properties of small-scale materials with the methods that are employed for bulk materials; probing micro/nano scale samples is challenged by the inherent difficulties associated with fabricating and handling of extremely small specimens.

In this presentation, I will introduce experimental studies utilizing micro/nano scale manufacturing to understand the mechanical behavior of thin films and to develop metallic alloys for metal MEMS applications. Measurements at elevated temperatures are performed through use of a custom-built in-situ SEM mechanical tester and two silicon-based micro heaters that support the sample and allow us to study the mechanical behavior of metallic thin films at temperatures up to 740 °C. Using this technique, I will present ongoing efforts in our laboratory utilizing the apparatus to understand the effect of an ultra-thin passivation layer on the mechanical behavior of sputter deposited nanotwinned Ni-Mo-W thin films.

11:10 - 11:40 16th, August

Ordered Nanoparticle Mediated Dislocation Transformation in Superalloys

Longsheng Feng, Michael J. Mills, and Yunzhi Wang

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High-temperature alloys in general and superalloys in particular are strengthened by ordered intermetallic phases that are relatively stable at elevated temperatures. Because of their low symmetry, these ordered intermetallic phases have rather complicated deformation mechanisms that are difficult to uncover by experiment alone. In this study we use a combination of ab initio calculation and phase field simulation at individual dislocation level to illustrate how the interactions between dislocations and precipitates of a low-symmetry ordered intermetallic phase such as gamma" (D0₂₂, tetragonal), the primary strengthening phase in IN718 superalloys, breed new particle dislocations, which may initiate twinning and other deformation modes. For example, two unstable stacking faults exist in gamma" phase, APB-like and CSF-like. These unstable stacking faults, once created, will transform spontaneously into nearby stable stacking faults on the generalized stacking fault (GSF) energy surface and generate new Shockley partial dislocations that do not exist in the system before the shearing events. Thus, the gamma" precipitates serve as a "dislocation-transformer" that transforms incoming <110>/2 dislocations into Shockley partials (<116>/6) that are not part of the incoming full dislocations. By passing the same <110>/2 dislocation consecutively on one slip plane from an active Frank-Reed source, we found that, for each type of <110>/2 full dislocations, only one specific Shockley partial prevails in the system. This could be one of the reasons why extensive micro-twinning is observed in these alloys. Understanding this precipitate-mediated dislocation transformation mechanism can further spark new ideas on alloy design, especially for tailoring the twinning mode. This work is supported by US NSF under the DMREF program (Grant No. DMR-1534826).

11:40 - 12:00 16th, August

Controlled Growth of Aluminum Nanowire Via Thermomigration Across a Nanoscale Junction

<u>Zhiyu Nie</u>

Mass transport driven by temperature gradient is commonly seen in fluids. However, by in situ transmission electron microscopy, we demonstrate that when drawing a cold nano-tip off a hot solid substrate (>300 $^{\circ}$ C), thermomigration can be so rampant that such mass transport mechanism can be exploited for producing single-crystalline aluminum, copper, silver and tin nanowires. This demonstrates that in nanoscale objects, solids can mimic liquids in rapid morphological changes, by virtue of fast surface diffusion across short distances. During uniform growth, a thin neck-shaped ligament containing a grain boundary (GB) usually forms between the hot and the cold ends, sustaining an extremely high temperature gradient that should have driven even larger mass flux, if not counteracted by the relative sluggishness of plating into the GB and the resulting back stress. This GB-containing ligament is quite robust and can adapt to varying drawing directions and velocities, imparting good controllability to the nanowire growth in a manner akin to Czochralski crystal growth.

14:00 - 14:30 16th, August

Atomistic Modeling of Hydrogen Diffusion and Hydrogen-enhanced Vacancy Diffusion in Metals

Shigenobu Ogata^{1,2,†}, Jun-Ping Du^{2,1}, Hajime Kimizuka¹, and Ju Li⁵

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We first present the theoretical estimates of the H and tritium diffusivities in face-centered cubic (fcc) Pd over a wide temperature range using the path integral first principles approach. Our approach exploits the temperature-dependent nuclear quantum effects (NQEs) of H diffusion in the metal (e.g., quantum fluctuations and tunneling), essential to quantitative characterizations of this subject—albeit largely omitted in previous models of H diffusion in fcc metals. We predicted the jump rates and diffusion coefficients of the H isotope in fcc Pd in a temperature range of 60–1500 K from first principles, while successfully considering NQEs based on Feynman's path-integral theory along with density functional theory (H. Kimizuka et al., Phys. Rev. B 97, 014102, 2018). Interestingly, we found that the temperature dependence of H-isotope diffusivities in fcc Pd has an anomalous 'reversed S' shape (i.e., it concaves down and up with an inflection point), in contrast to the familiar 'C' shape (i.e., it concaves up at a crossover temperature), on the Arrhenius plots.

Next, we study the vacancy diffusion in metals with hydrogen environment. Hydrogen atoms bind strongly to vacancy, and often believed vacancy diffusion slows down. Here, we studied the effect of varied number of adsorbed H at the saddle-point on the vacancy diffusion using the atomistic simulations in face-centered cubic Cu. At the low H-concentrations corresponding to the low chemical potential of H, where an assumption of the constant number of absorbed H at the saddle-point is valid, we found that although the trapped H tends to increase the vacancy diffusion barrier, nontrapped environmental H tends to reduce it, and both trapped and nontrapped H enhance the frequency of vacancy jumping attempts based on the harmonic TST. Altogether, vacancy diffusion is slightly accelerated. On the contrary, at high H-concentration due to high chemical potential of H, the direct MD simulations show H-atoms significantly enhance the vacancy diffusion due to a positive hydrogen Gibbs excess at the saddle-point: that is, the migration attracts more H than the vacancy ground state. Thus, according to generalized Gibbs adsorption isotherm, higher chemical potential of H significantly lowers the migration free-energy barrier.

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14:30 - 15:00 16th, August

Understanding The Hydrogen Embrittlement by Novel Critical Experiments

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Hydrogen embrittlement is a complicated process hard to investigate due to the volatile nature of the hydrogen atom and different states it can exist in the metals. Therefore, to reveal the underlying mechanism of the hydrogen embrittlement, we designed and performed "critical experiments." In this paper, we will present some of our novel approaches used to study the hydrogen embrittlement in different alloy systems. We specifically used in situ hydrogen charging combined with nanoindentation, microcantilever bending, and tensile testing to observe the hydrogen embrittlement at various microstructural length scales. Additionally, we used high-resolution microstructural characterization techniques including. High-resolutionElectron Backscattered Diffraction (EBSD), Electron Channeling Contrast Imaging (ECCI), transmission EBSD (t-EBSD) and Transmission Electron Microscopy.

15:00 - 15:30 16th, August

Hydrogen Effect on The Evolution of Microstructure at High Strain Level

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In order to understand the hydrogen effect on the microstructure evolution processes and its relation to the hydrogen-induced fracture mode transition, the microstructures in hydrogen-charged pure nickel after high-pressure torsional processing and a ferritic-pearlitic low carbon steel fatigued in a 40MPa hydrogen gas environment were investigated. Electron transparency foils were extracted from sites of interest by using focused-ion beam, and the microstructures were examined under zone-axis bright-field imaging condition in a scanning transmission electron microscope. The local crystalline orientations were obtained by using automated crystal orientation mapping technique. In comparison to the structure formed in air, the size of the dislocation structure unit was refined, and the misorientation angle gradient was modified by hydrogen. A general law for the evolution of microstructure and failure process at a high strain level in the presence of hydrogen was proposed.

15:30 - 15:55 16th, August

Hydrogen Effect on Defect kinetics–A Generalized Gibbs Isotherm Theory

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Vacancy diffusion is fundamental to materials science. Hydrogen atoms bind strongly to vacancy, and were often believed to retard vacancy diffusion. Here, we use potential-of-mean-force method to study the diffusion of vacancy in Cu and Pd. We find H-atoms, instead of dragging, enhance the diffusivity of vacancy due to a positive hydrogen Gibbs excess at the saddle-point: that is, the migration attracts more H than the vacancy ground state, characterized by an activation excess $\Gamma_{\rm H}^{\rm m} \sim 1$ H, together with positive migration activation volume $\Omega^{\rm m}$ and activation entropy $S^{\rm m}$. Thus, according to generalized Gibbs adsorption isotherm, higher $\mu_{\rm H}$ significantly lowers the migration free-energy barrier. This is verified by direct molecular dynamics simulations. This trend is believed to be generic for migrating dislocations, grain boundaries, etc. that have higher capacity for attracting H due to positive activation volume at the migration saddle-point.

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15:55 - 16:20 16th, August

Hydrogen Embrittlement of High Manganese Steel Examined by Small-scale Testing

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High manganese steels have received much interest in recent years due to their outstanding mechanical properties combining high strength and good ductility. However, this material group is susceptible to unexpected mechanical degradation when exposing to hydrogen containing environments due to hydrogen embrittlement. The volatile nature of hydrogen atoms and different existing states in metals makes hydrogen embrittle a complicated process that difficult to investigate. Therefore, we performed small scale mechanical tests in hydrogen containing environment to reveal the underlying mechanism. In this paper, we will present our novel studies of hydrogen charging nanoindentation and tensile test with in-situ scanning electron microscope (SEM) observation. Additionally, the characterization techniques of high-resolution electron backscattered diffraction (EBSD) and electron channeling contrast imaging (ECCI) and simulation models were used to evaluate the effect of hydrogen.

Keywords: Hydrogen embrittlement; Electrochemical nanoindentation; Tensile test; TWIP steel; In-situ test

16:20 - 16:40 16th, August

Hydrogen Effects on The Motion of Screw Dislocation in α- iron

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Hydrogen embrittlement (HE) has been known as a longstanding threat to the integrity and safety in structural metals, among which iron and steels attract the most attention because of their wide application in manufacturing industry and infrastructure. Uncovering the interaction between hydrogen and dislocation is essential for comprehending the underlying HE mechanisms. Here by carrying out in situ quantitative mechanical testing on individual screw dislocations in a submicron sized α -Fe pillar in an state of the art environmental transmission electron microscope, we demonstrate that the behaviors of screw dislocations can be largely altered by hydrogen. When the sample exposed to a 2 Pa level hydrogen, the activation stress of an individual dislocation with two fixed-ends is lowered remarkably and the forward-march distance of the forward-and-back type motion is markedly enlarged under the same-peak-force cyclic loading. In addition, the effects on dislocation movements are reversible after the hydrogen gas cut off. More detailed analysis on dislocation behavior associated with hydrogen is discussed. These findings offer quantitative information for understanding the hydrogen-affected microstructural evolution in the plastic deformation.

Appendices

Xi'an Jiaotong University

Xi'an Jiaotong University (abbreviated XJTU) is a Chinese C9 League university with strengths in engineering, technology, and public health located in Xi'an, Shaanxi, China. XJTU is a top university in China, affiliated to the Chinese Education Ministry, and is one of the oldest current institutions of higher education in China. XJTU is composed of 10 branches of learning, namely, science, engineering, medicine, economics, management, literature, law, philosophy, education and art, which is divided into 26 full-time colleges and schools. XJTU boasts a high-level staff of over 5,500, including 3000 full-time teachers, among which are 1,800 professors and associated professors. XJTU has over 32000 full-time registered students with half of them being graduate students. 1800 of them are internationals students. The university has an extensive system of scholarships and stipends, with scholarships for undergraduates totaling 12 million Yuan per year, and additional annual support in the form of loans totaling 14.4 million Yuan. The university has also established an "innovation fund" to provide support for graduate students. Each year, it distributes about 50 million Yuan.



XJTU grew out of Nanyang College, which was founded in 1896 in Shanghai and renamed Jiaotong University in 1921. In 1956, the main body of Jiaotong University was moved to Xi'an according to the decision issued by the State Council, and was formally named Xi'an Jiaotong University in 1959 which was listed as a national key university. Xi'an Jiaotong University, as one of the first universities entering the seventh and eighth five-plan, as well as China's "211 Project" and "985 Project", is selected to be developed into a global first-class university. In April 2004, approved by the State Council, the original Xi'an Medical University and original Shaanxi Institute of Finance and Economics were integrated into Xi'an Jiaotong University.

Xi'an Jiatong University, which is located in the city of Xi'an in Shaanxi province, has three campuses: the Xingqing campus, the Yanta campus and the Qujiang campus, covering a total area of 1.9894 million square meters. The total constructed area is 2.0385 million square meters. The "Qian Xuesen Library," named after alumnus Qian Xuesen, which is authorized by the Propaganda Department of the CPC, and whose name was rendered by Jiang Zemin, is located on the Xingqing campus, covering

nearly 40 thousand square meters and has 3,518 reading seats. The library collections include 5.0701 million books and 10,053 newspapers and periodicals, of which 4,089 types are current periodicals. The library has also been improving its digital collections, and has recently introduced 252 foreign electronic resources. Its holdings now include 28,639 electronic periodicals in Chinese and foreign languages and more than one million electronic books and 1.07 million e-books and 15 kinds of world famous periodicals covering more than one hundred years. The library's computer system is fully integrated with the campus network, CERNET, and the Internet. On and off-campus users have access to the system via remote terminal or over the Internet. The university's computer network meets the highest international standards. Students are housed in modern dormitories and may choose from a wide variety of dishes in the university's extensive dining facilities. The Siyuan Student Activities Center, with a total area of over 10,000 square meters, is the venue for a variety of events, and the university's athletic fields and playgrounds are modernly equipped. The university has a modern psychological health education and counseling center for college students.

School of Materials Science and Engineering

School of Materials Science and Engineering (MSE) of Xi'an Jiaotong University was founded in 2002. MSE has three departments, including Department of Material Science, Department of Materials Processing Engineering and Department of Physics and Chemistry, and more than 10 Research Centers Institutes and Laboratories, equipped with excellent infrastructures and state-of-the-art facilities. MSE operates and co-operates two national-level research institutions, namely, State Key Laboratory for Mechanical Behavior of Materials (SKL-MBM), and International Joint Laboratory for Micro/Nano Manufacturing and Measurement Technologies (IJL-MMMT). MSE is the key construction discipline supported by National "211 Project" and "985 Project" of China. It is always one of the best disciplines in assessments by Ministry of Education of China, and MSE was granted as the National Key Discipline in 2007. MSE has a strong faculty comprised of over 100 faculty members and technicians, including 55 professors/associate professors, and has around 1200 students, including 250 PhD students, 450 Master students and around 500 Bachelor students.



In the past decade, MSE has achieved fruitful results, and has contributed to the development of national economy significantly. MSE has been in charge of 3 "Basic Research Plan of China" 973 projects, 1 key 863 project supported by "National High Technology Research and Development Program" and more than 600 other research projects supported by the National Natural Science Foundation of China (NSFC), National Ministries and Commissions and Enterprise Collaboration. MSE has won many outstanding awards, including 1 Second Prize of National Natural Science, 5 Second Prize of National Award for Technological Inventions, 1 Second Prize for National Scientific and Technological Progress, more than 20 Science and Technology Awards of Shaanxi Province or Ministry of Education. They published more than 2000 papers indexed in SCI, including more than 60 high-profile research papers, published on Nature, Science, Nature Materials, Nature Photonics, Nature Communications, Advanced Materials, Nano Letters, Physical Review Letters,

Angew. Chem. Int. Ed., J. Am. Chem. Soc., PNAS and so on. Moreover, MSE owns more than 300 authorized patents. MSE has established world-wide collaborations for research development and international exchange programs with foreign countries and regions abroad, like, USA, France, Germany, Japan, South Korea, and so on. Tens of international research centers were established and attracted excellent scholars and teams from worldwide. MSE entered the "International Top 50 Disciplines".

CAMP-Nano

The Center for Advancing Materials Performance from the Nanoscale (CAMP-Nano) was established in 2009. It is endowed with cutting-edge instruments, and powered by fun-loving and exploratory spirits, which make us a creative and happy team, an envied home. Campers strive to be pioneers at the frontiers of nanoscience and nanotechnology. Having enjoyed the camp life here, campers will become leaders in academia, industry or business.

As a research group, CAMP-Nano has published more than 150 papers since 2010, including many papers in the most prestigious journals, such as Nature (2), Science (2), Nature Materials (3), Nature Communications (10), PNAS (2), Physical Review Letters (2), Advanced Materials (1), Nano Letters (10) et al.

Until now CAMP-Nano has attracted ten outstanding young talents for full-time faculty positions. All of them have great overseas research credentials. To keep the advanced facilities running at their best performance, CAMP-Nano has appointed ten high-level technicians and four administrative secretaries. And up to now, 86 students (27 PhD candidates and 59 master students) have joined us.

Besides, CAMP-Nano has been cooperating with many other research groups and companies around the world. Till now, two other centers, Hysitron Applied Research Center in China (HARCC) and XJTU-HHT Research and Development Center (XHRDC), collaborated with Hysitron and Hitachi High-Technologies respectively, have been established. At the end of 2015, Engineering Research Center for Magnesium-based New Materials was founded. It is equipped with complete equipments for material preparation, processing and characterization in recent years. The center has made many breakthroughs in the theory of plastic deformation of magnesium alloys, the design and preparation of magnesium alloys, the refining of high-purity magnesium and the smelting technology of raw magnesium.

The laboratory of CAMP-Nano has acquired and developed first-class instruments valued at about 10,000,000 US dollars. Most of these are first of their kind, not only in China but also in Asia and the world. However, CAMP-Nano not only conducts innovative research projects based on these state-of-the-art scientific instruments (see below), but also hopes to accelerate the translation of basic scientific knowledge into industrial applications by bridging the scientific community and technological companies.



Hitachi H-9500 300 kV Environmental TEM In situ atomic resolution imaging with gas injection and sample heating



Hitachi SU6600 FESEM Advanced variable pressure technology and an improved Schottky field emission electron source



JEOL JEM-2100F HRTEM In situ mechanical and electrical testing with Hysitron PI 95 and PI 95 ECR; equipped with EELS, EDS and another two Gatan CCD cameras



FEI Helios NanoLab 600 DualBeam FIB In situ mechanical testing with Hysitron PI 85; equipped with EBSD, EDS and Kleindiek micromanipulator



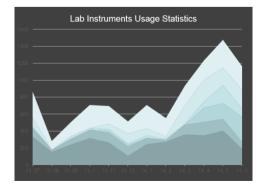


NanoDMA III



MultiRange NanoProbe

The Hysitron **TI 950 TriboIndenter** is the next generation nanomechanical test instrument providing industry-leading sensitivity and unprecedented performance.



The Smart Laboratory Management Online System

All the facilities in CAMP-Nano are available to our center users through the EASY-LAB online system. Users can register, reserve and arrange their experiments by logging onto this system from their smart phone or computer. Additionally, the lab manager at CAMP-Nano automatically gets real-time functional information of equipments during their operation.

Xi'an Tour Guide

The continuous history of Xi'an has apparently resulted in its magnificent culture. Today's Xi'an is a world famous tourist city and an inexhaustible treasure house of cultural relics. Now heads of state from many countries and people from all walks of life come to the city to broaden their knowledge of Chinese civilization.



Foremost is the China's greatest archeological excavation, the Terra Cotta Warriors and Horses. Life size terracotta figures of warriors and horses arranged in battle formations symbolically guard the Mausoleum of Emperor Qin Shi Huang, the first emperor of the Qin dynasty (246-209B.C). The State Council authorized the building of a museum on the site in 1975 for the protection of the discovery. So far, altogether over 7,000 pottery soldiers, horses, chariots, and even

weapons have been unearthed and displayed in the museum. It is cited as the 'Eighth Wonder of the World' and was listed by UNESCO in 1987 as one of the world cultural heritages.

Spending some time at the **Huaqing Hot Springs** on the way back from the Terra Cotta Army site is a must for every visitor to Xi'an. For centuries emperors came here to bathe and enjoy the scenic beauty, and it has been a favorite spa since the Tang Dynasty (618-907 A.D). The palace complex has also been the scene of political intrigue, so there is plenty of interest to discover during your visit.

Covering an area of about 100,000 square meters, **the Banpo Village Remains** was a village settlement of the earliest inhabitants of Xi'an, typical of the Neolithic Yangshao culture. At this site, archaeologists have discovered nearly 10,000 production tools and daily utensils of various kinds and the remains of 45 houses, 200 cellars, 6 pottery kilns, 174 adults' burial pits and 73 children's burial jars.

Every Ming city (1368-1644) had **a bell** tower and a drum tower. The bell was sounded at dawn and the drum at dusk. The two buildings at Xi'an are the best known in China. The Bell Tower was built in the city center and from the top can enjoy a panoramic view of the whole of Xi'an. Not far away to the west is the Drum Tower, a large drum inside was for marking the passage of time each night in ancient times. Now, they are



outstanding examples of the ancient architecture of Xi'an.

Housing more than 2,300 famous steles and inscribed memorial tablets of the Han, Wei, Sui, Tang, Yuan, Ming, Qing dynasties and known as the largest 'stone-book warehouse' in China, **the Forest of Stone Steles** in Xi'an is a treasure house of calligraphic art. It is situated on Sanxue Jie, near the south gate of the Xi'an City Wall. **The City Wall** in Xi'an is the most complete city wall to survive in China, as well being one of the largest ancient military defensive systems in the world. It was built first in the early Ming Dynasty (1368-1644) and renovated in recent years. Outside the city wall is a moat. A circular park has now been built along the high wall and the deep moat.

Additional attractions are the **Big Wild Goose Pagoda and Small Wild Goose Pagoda of the Tang Dynasty** (618-907 A.D), while worshipers still frequent the Great Mosque and the famous Famen Temple noted for its collection of Sakyamuni's relics. These together with the magnificent Shaanxi History Museum are all highly recommended attractions to be visited when you come to Xi'an.

Xi'an Jiaotong University, a national key university under the direct jurisdiction of the Ministry of Education, is one of the country's oldest institutions of higher learning. Founded in Shanghai in 1896 as Nanyang Public, it was renamed Jiaotong University in 1921. In 1956, at the direction of the State Council, the university was moved to Xi'an, and renamed Xi'an Jiaotong University (XJTU). As one of the country's national key universities, it was included in the first group of universities singled out for high priority development under the country's seventh and eighth five year plans. It was also included in the first group of universities to benefit from Project 211 and Project 985, with the goal of becoming a world class university.



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