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First International Conference on Heterostructured Materials (HSM I)

12 - 15 July 2022, Hong Kong, China

Conference website:
https://www.hkias.cityu.edu.hk/event/first-international-conference-on-heterostructured-materials/

First International Conference on Heterostructured Materials (HSM I)

12 - 15 July 2022

Lecture Theatre

Hong Kong Institute for Advanced Study

LG/F, Academic Exchange Building

City University of Hong Kong

Committee

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Liliana Romero Reséndiz	Postdoctoral Researcher, Department of Materials Science and Engineering, City University of Hong Kong, China

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City University of Hong Kong

<u>Day 1, 12 July 2022 (Tuesday)</u>

Time (GMT +8)	Activity	Modality
9:00 – 9:10	Opening ceremony	Onsite
Session 1: Heterostructured materials: Mechanical behavior I **Session Chair: Yuntian Zhu, City University of Hong Kong**		
9:10 – 10:00 Plenary	**Huajian Gao** (Nanyang Technological University, Singapore) *Engineer metals with internal interfaces for enhanced mechanical performance*	Online
10:00 – 10:30 Invited	**Amit Misra** (University of Michigan, USA) *Plasticity in Laser Processed Al-Si Eutectic Alloys*	Online
10:30 – 10:50	Break	
10:50 – 11:20 Invited	**Xinghang Zhang** (Purdue University, USA) *Mechanical behavior of nanostructured metallic materials with thick grain boundaries*	Online
11:20 – 11:50 Invited	**Zhaohua Hu** (Ansteel Beijing Research Institute Company, China) *Industrial manufacturing of Heterogeneous Materials: Preliminary investigation and perspectives*	Online
11:50 – 12:10	**Zhaoxuan Wu** (City University of Hong Kong, China) *The cores of the screw dislocations in BCC transition metals and alloys*	Onsite
12:10 – 14:00	Lunch	
Session 2: Heterostructured materials: Mechanical behavior II **Session Chair: Yang Lu, City University of Hong Kong**		
14:00 – 14:40 Keynote	**Jacob Huang** (City University of Hong Kong, China) *Quantifying the hetero-deformation induced strengthening in bimodal grain structure*	Online
14:40 – 15:20 Keynote	**Hao Zhou** (Nanjing University of Science and Technology, China) *Dislocation mechanisms of HDI hardening in heterostructured materials*	Online
15:20 – 15:50 Invited	**Guohua Fan** (Nanjing Tech University, China) *Deformation behaviors of layered metallic materials revisited from local stress and local strain*	Online
15:50 – 16:20 Invited	**Xinkun Zhu** (Kunming University of Science and Technology, China) *Strain hardening behavior and microstructure evolution of gradient-structured Cu-Al alloys with low stack fault energy*	Online
16:20 – 17:10	Break	

Time (GMT +8)	Activity	Modality
17:10 – 17:40 Invited	**Heinz Werner Höppel** (Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany) *Understanding the role of heterostructured phase boundaries in copper-based lamellar metallic composites*	Online
17:40 – 18:00	**Sergey Zherebtsov** (Belgorod State University, Russia) *Microstructure and mechanical properties of Ti-Nb-Zr alloy-based composites, reinforced by boride particles*	Online

Day 2, 13 July 2022 (Wednesday)

Time (GMT +8)	Activity	Modality
Session 3: Design of new heterostructured materials Session Chair: Yang Ren, City University of Hong Kong		
9:00 – 9:40 Keynote	**Irene J. Beyerlein** (University of California, USA) *Thick alloy interfaces in metallic nanolaminates*	Online
9:40 – 10:10 Invited	**Yunzhi Wang** (Ohio State University, USA) *Creating compositional and structural heterogeneities for controlled strain release during deformation*	Online
10:10 – 10: 30	Break	
10:30 – 11:10 Keynote	**Kei Ameyama** (Ritsumeikan University, Japan) *Harmonic Structure: a novel HSM design for outstanding mechanical properties*	Online
11:10 – 11:50 Keynote	**Suveen Mathaudhu** (Colorado School of Mines, USA) *Synthesis and nanoscale heterogeneity mapping of amorphous/crystalline laminated metals*	Online
11:50 – 12:20 Invited	**Andrea Hodge** (University of Southern California, USA) *Heterogeneous nanostructured in nanotwinned inconel alloys*	Online
12:20 – 14:00	Lunch	
Session 4: Trends in heterostructured materials Session Chair: Yong Yang, City University of Hong Kong		
14:00 – 14:40 Keynote	**Yuri Estrin** (Monash University, Australia) *Architectured materials: trends and perspectives*	Online
14:40 – 15:20 Keynote	**Xiuyan Li** (Shenyang National Laboratory for Materials Science, China) *Schwarz crystal in metals*	Online
15:20 – 15:50 Invited	**Guilin Wu** (University of Science and Technology Beijing, China) *Achieving high strength and large elongation in steels via heterogeneous structure design*	Online
15:50 – 16:10	Break	
Session 5: Multifunctional heterostructured materials Session Chair: Yong Yang, City University of Hong Kong		
16:10 – 16:50 Keynote	**Xiangyi Zhang** (Yanshan University, China) *Engineering ordered heterostructured materials with ultrahigh energy density*	Online
16:50 – 17:10	**Anding Wang** (Dongguan University of Technology, China) *Heterostructured Fe-Based alloys with unprecedented soft-magnetic properties and manufacturability*	Online
17:10 – 17:30	**Jianguo Li** (Northwestern Polytechnical University, China) *Investigations on ballistic impact performance of gradient structured AZ31 Mg alloy with enhanced strength and plasticity*	Online
Evening	Banquet	

Day 3, 14 July 2022 (Thursday)

Time (GMT +8)	Activity	Modality
Session 6: Simulation of heterostructured materials **Session Chair: Yuntian Zhu, City University of Hong Kong**		
9:00 – 9:20	**Marc Andre Meyers** (University of California San Diego, USA) *The role of pre-existing heterogeneities in copper under shock*	Online
9:20 – 9:50 Invited	**Caizhi Zhou** (University of South Carolina, USA) *Atomistic analysis of shear band formation in metallic nanolayered composites*	Online
09:50 – 10:50	Break	
10:50 – 11:10	**Hyoung Seop Kim** (Pohang University of Science and Technology, South Korea) *Microstructural features in bimodal structure-property linkage*	Online
11:10 – 11:30	**Jianfeng Zhao** (China Academy of Engineering Physics, China) *Multiscale modeling of heterostructured materials*	Online
11:30 – 11:50	**Xu Zhang** (Southwest Jiaotong University, China) *Multiscale discrete dislocation dynamics study of gradient nano-grained materials*	Online
11:50 – 13:30	Lunch	
Session 7: High/medium entropy alloys-1 **Session Chair: Zhaoxuan Wu, City University of Hong Kong**		
13:30 – 13:50	**Xiaozhou Liao** (University of Sydney, Australia) *Manipulation of gradient structure profile in a CrMnFeCoNi high-entropy alloy for superior mechanical properties*	Online
13:50 – 14:20 Invited	**Jae Bok Seol** (Gyeongsang National University, South Korea) *Thermally and mechanically induced hererogenity in high-entropy alloy: short – range order*	Online
14:20 – 14:40	**Xiaochong Lu** (Sichuan University, China) *Gradient structured high entropy alloy with improved synergy of strength and ductility: experiments and crystal plasticity simulations*	Online
14:40 – 15:00	**Guodong Li** (Beihang University, China) *Simultaneously enhanced strength and strain hardening capacity in high-entropy alloy via harmonic structure design*	Online
15:00 – 15:20	**Yong Yang** (City University of Hong Kong, China) *Novel heterogeneous lattice strain strengthening in severely distorted crystalline solids*	Online
15:20 – 15:40	**Feng He** (Northwestern Polytechnical University, China) *Strain partitioning enables excellent tensile ductility in precipitated heterogenous high-entropy alloys with gigapascal yield strength*	Online
15:40 – 16:00	Break	

Time (GMT +8)	Activity	Modality
Session 8: High/medium entropy alloys-2 **Session Chair: Zhaoxuan Wu, City University of Hong Kong**		
16:00 – 16:30 Invited	**Zhangwei Wang** (Central South University, China) *Characterize microstructures of heterostructured high-entropy alloys via correlative EBSD and ECCI*	Online
16:30 – 17:00 Invited	**Fuping Yuan** (University of Chinese Academy of Sciences, China) *Mechanical properties and deformation mechanisms in high entropy alloys with dual heterogeneous/graded structures*	Online
17:00 – 17:20	**Yang Lu** (City University of Hong Kong, China) *High-entropy alloy microlattice metamaterials*	Onsite
17:20 – 17:40	**Qingsong Pan** (Shenyang National Laboratory for Materials Science, China) *Gradient-cell-structured high-entropy alloy with exceptional strength and ductility*	Online
17:40 – 18:00	**Tao Yang** (City University of Hong Kong, China) *Heterogenous columnar-grained high-entropy alloys produce exceptional resistance to intermediate-temperature intergranular embrittlement*	Online

Day 4, 15 July 2022 (Friday)

Time (GMT +8)	Activity	Modality
Session 9: Microstructural mechanism of heterostructured materials-1 Session Chair: Yong Yang, City University of Hong Kong		
9:00 – 9:50 Plenary	**David Srolovitz** (University of Hong Kong, China) *Predictive Microstructure Evolution*	Onsite
9:50 – 10:30 Keynote	**Darcy A. Hughes** (Fremont, USA) *Gradient bulk nanostructures with exceptional strength*	Online
10:30 – 10:50	Break	
10:50 – 11:30 Keynote	**Xiaoxu Huang** (Chongqing University, China) *Heterostructured metallic materials: multiscale and multidimensional characterization and tailoring of the microstructure and properties*	Online
11:30 – 12:10 Keynote	**Gang Liu** (Xi'an Jiaotong University, China) *Freezing solute atoms in nanograined aluminum alloys via high-density vacancies*	Online
12:10 – 13:50	Lunch	
Session 10: Microstructural mechanism of heterostructured materials-2 Session Chair: Liliana Romero Reséndiz, City University of Hong Kong		
13:50 – 14:30 Keynote	**Yang Ren** (City University of Hong Kong, China) *On the structural origins of novel properties of some heterostructured materials*	Onsite
14:30 – 15:00 Invited	**Hongwang Zhang** (Yanshan University, China) *Ultrahard twinned substructure induced by martensitic transformation in steels*	Online
15:00 – 15:30 Invited	**Andy Godfrey** (Tsinghua University, China) *In-situ investigation of local plastic deformation in aluminum with near-micrometer grain size and heterogeneous grain-size distribution and arrangement*	Online
15:30 – 15:50	Break	
Session 11: Effects of interfaces in heterostructured materials Session Chair: Yuntian Zhu, City University of Hong Kong		
15:50 – 16:30 Keynote	**Yueguang Wei** (Peking University, China) *The effects of interface and plastic strain gradient in heterostructured metals*	Online
16:30 – 17:10 Keynote	**Yuntian Zhu** (City University of Hong Kong, China) *Effects of hetero-zone interaction on strain accommodation in heterostructured materials*	Online
17:10 – 17:40 Invited	**Deliang Zhang** (Northeast University, China) *The nature and roles of heterogeneous structures in sustaining high strength-ductility synergy in PM titanium and titanium alloys*	Online
17:40 – 18:00	**Yuanshen Qi** (Guangdong Technion-Israel Institute of Technology, China / Technion-Israel Institute of Technology, Israel) *Manipulating three- and zero-dimensional defects in heterostructured gradient materials*	Online

Online content

Tutorial: "Introduction to Heterostructured Materials"

Yuntian Zhu (City University of Hong Kong, China)
HSM I website, "tutorial" section.
https://www.hkias.cityu.edu.hk/event/first-international-conference-on-heterostructured-materials/

Poster session

HSM I website, "poster exhibition" section.

Corresponding author	Title	Contact for further questions or comments
Ahmed Dawelbeit (Donghua University, China)	*Transient Confinement of the Quaternary Tetramethylammonium Tetrafluoroborate Salt in Nylon 6,6 Fibres: Structural Developments for High-Performance Properties via a Temporal Weakening of the Hydrogen Bonds*	amsdawelbeit@yahoo.com
Sang Guk Jeong (Pohang University of Science and Technology, Republic of Korea)	*Fabrication of heterogeneous layered structure with selective laser melting additive manufacturing*	san.jeong@postech.ac.kr
Yang Liu (Zhengzhou University, China)	*Effect of Al2O3 doping on microstructure evolution and densification process of AZO targets*	louis@zzu.edu.cn
Yan Ma (City University of Hong Kong, China)	*Ultra-high tensile strength via precipitates and enhanced martensite transformation in a FeNiAlC alloy*	yanma24@cityu.edu.hk
Dafaalla Mahjoub Dafaalla Babiker (University of Science and Technology of China, China)	*Effects of electron beam irradiation crosslinking on microstructure and electrochemical performance of hybrid polyethylene separators for lithium-ion batteries*	dafaalla@mail.ustc.edu.cn
Maxim Ozerov (Belgorod State University, Russia)	*Effect of hardening with borides on the microstructure and mechanical properties of Al5Nb24Ti40V5Zr26 alloy-based composites*	ozerov@bsu.edu.ru
Evgeniya Panina (Belgorod State University, Russia)	*Mechanical propertied and deformation behavior of novel refractory high-entropy alloys with a BCC-B2 structure*	panina_e@bsu.edu.ru
Elizaveta Povolyaeva (Belgorod State University, Russia)	*Formation of a heterogeneous microstructure in a medium entropy alloy of the Fe-Co-Ni-Cr-C system*	povolyaeva@bsu.edu.ru
Sara Saad (Belgorod State University, Russia)	*Cold sintering of electronic materials*	sara.saad@aims-senegal.org
Anastasiia Semenyuk (Belgorod State University, Russia)	*The effect of nitrogen on the structure and mechanical properties of the Fe40Mn40Cr10Co10-based alloys*	semenyuk@bsu.edu.ru
Nikita Stepanov (Belgorod State University, Russia)	*Microstructure and mechanical behavior of Al-doped CoCrFeMnNi with dual-phase FCC/B2 structure*	stepanov@bsu.edu.ru
Zuohua Wang (Yanshan University, China)	*{112}<111> Twins or twinned variants induced by martensitic transformation?*	zhwang@stumail.ysu.edu.cn

Huajian Gao

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Engineer metals with internal interfaces for enhanced mechanical performance

Gradient microstructures with internal interfaces exist ubiquitously in nature and are increasingly being introduced in next generation engineering materials with unprecedented mechanical properties. Here we discuss some recent studies on engineering metals with nature-inspired internal interfaces and gradients. First, metals typically suffer from cumulative, irreversible damage to microstructure during cyclic deformation, leading to limited fatigue life along with cyclic responses that are unstable and history-dependent. Through atomistic simulations and variable-strain-amplitude cyclic loading experiments at stress amplitudes lower than the tensile strength of the metal, we report a history-independent and stable cyclic response in bulk copper samples with microstructures mimicking the highly oriented nanoscale twin boundaries in conch shells. We demonstrate that this unusual cyclic behaviour is governed by an unusual type of dislocations called correlated 'necklace' dislocations (CNDs). Furthermore, we show that introducing gradient nanotwinned structure in metals results in extra strengthening that defies the classical rule of mixture theory. This phenomenon is attributed to another new type of dislocations called bundles of concentrated dislocations (BCDs).

David Srolovitz

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Predictive Microstructure Evolution

The control of microstructure evolution is central to the development of heterostructured materials. Most microstructure evolution is controlled by interface motion; hence, understanding and quantitative prediction of interface migration is a universal goal of materials science. How interfaces migrate is, in turn, dependent on interface structure and, more precisely on the defects that define interface structure and how they migrate. These defects are disconnection; i.e., line defects with both step and dislocation character that are constrained to lie in the interface and which can be defined in terms of interface bicrystallography. In this presentation, we review what is known about disconnections and how they move, interact and give rise to interface migration. Since it is not practical to account for every disconnection on every interface in the microstructure, we introduce a continuum model for microstructure evolution that accounts for bicrystallography and the disconnection-based mechanism for interface migration. We apply the resultant continuum model in both sharp interface and diffuse (phase field) simulations of the evolution of individual grains/particles as well as polycrystalline and multiphase microstructures. We also discuss the effects of interface anisotropy along with capillarity, chemical potential, and stress-driven microstructure evolution.

Kei Ameyama

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Harmonic Structure: a novel HSM design for outstanding mechanical properties

The present talk is aimed at providing a critical assessment of the novel concept of Harmonic Structure design, and identifying and discussing key issues that deserve additional studies. The harmonic structure is a recently introduced concept to paves the way for engineering metallic materials with excellent mechanical performance. They consist of soft coarse-grained regions (Core) that are three-dimensionally surrounded by a connected network of hard ultra-fine grained regions (Shell). The interaction in these Core-Shell regions produces a synergistic effect, during plastic deformation, leading to superior mechanical properties that are extremely important in practical applications. Although the harmonic structure material is a hetero-structure material, it deforms more uniformly than conventional materials, resulting in high ductility and toughness while achieving high strength. This is achieved by work hardening due to dislocation generation, accumulation, and movement in the nanoscale region and large uniform deformation due to suppression of deformation localization in the macroscale region. This is the result of the superposition of nanoscale and macroscale microstructure and mechanical properties. In addition, stress concentration in shells can cause selective phase transformation and recrystallization even in small deformations, and in the process of microstructure formation from nanocrystalline grains, not only grain size gradients but also constituent phase gradients due to elemental distribution are generated. In addition, HS materials also demonstrate good wear and corrosion properties. These unique phenomena create a synergy between nano- and macro-scale phenomena, which is the goal of nano-engineering, and lead to the development of innovative mechanical properties that are extremely important in practical applications. There is a possibility that there are still many unknown phenomena between nano and macro scales, and it is highly expected that the elucidation of these unique phenomena will lead to new material innovations.

Irene Beyerlein

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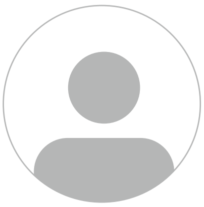
Thick alloy interfaces in metallic nanolaminates

Even after their introduction some decades ago, metallic nanostructured, multi-phase composites have continued to draw world-wide interest due to their exceptionally high strength and hardness and outstanding tolerance to extreme conditions, such as elevated temperatures, irradiation, and high-rate impact. The combination makes them an exciting class of materials for meeting the demands of future applications, such as nuclear power reactors, propulsion systems, and microelectromechanical devices. At present, however, they are not suitable for long-time service due to insufficient toughness and a greater tendency to develop shear localizations than their more coarsely structured counterparts. A unique and important feature of these materials is the physical dominance of biphase interfaces, the atomically thick boundary between the dissimilar phases in the composite. The deformation response of the biphase interface and interactions with moving dislocations can have a profound effect on overall material behavior, suggesting the appealing potential to control its localization tendencies via design of the interface itself. In this talk, we will focus on the behavior of nanolayered nanocomposites made with extraordinarily “thick” interfaces under mechanical deformation. We will discuss efforts to characterize and design the morphology, size, and chemistry of the interface, especially in its third dimension (normal to the interface plane). Results from a model developed to simulate the dynamic interactions of individual dislocations and these 3D interfaces under applied stress will be presented. The talk will share our findings to date, which indicate that both the macroscopic and microscopic responses are sensitive to interface thickness and through-thickness chemical gradients. We will conclude with a discussion on the intriguing possibility to design 3D thick interfaces to attenuate shear concentrations and postpone instabilities without sacrificing strength.



Ruqing Cao

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Preparation and characterization of gradient grained nickel

Gradient structured (GS) materials are ubiquitous in biological systems and now increasingly adopted in engineering systems to achieve desirable combinations of mechanical properties. In the present work, pure Ni samples possessing a gradient structure with a change in the grain size up to three orders of magnitude as well as various degree of grain size gradient is accurately controlled were prepared by electrodeposition. The GS Ni samples exhibit a favorable combination of high strength and high ductility. An optimal grain size distribution profile is discovered. Experimental observations and molecular dynamics (MD) simulations reveal that the surface roughening of coarse grains and strain localization of nano-grains can be effectively suppressed by the mutual constraint between nano-grains and coarse grains, leading to the observed superior uniform elongation. This work not only reports a promising methodology of producing materials possessing both high strength and high ductility, but also provides a model for investigating the deformation mechanisms in GS materials.

Yuri Estrin

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Architectured material: trends and perspectives

This talk addresses some trends in design of architectured materials. While the areas to be discussed are somewhat outside of the main theme of this conference, some ideas of architecturing materials at meso scale we outline are related to it. The subjects to be covered include topological interlocking materials, lattice materials, and lithomimetics. Their inner architecture at meso scale is a key factor impacting on the material properties. We present the principles governing the design of the emerging materials architectures, discuss their explored and anticipated properties, and give an outlook on their future developments and applications.

Chongxiang Huang

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Effects of hetero-zone interaction on strain accommodation in herterostructured materials

Herterostructured materials, as a new class of materials, have captured much attention during the past decade due. Different from the addition of alloy elements, the charm of herterostructured materials is that tuning the size, shape and distribution of domains can yield unprecedented mechanical behaviors, such as "1+2>3" effect on strength, work hardening and uniform elongation [1-3]. The key mystery lies on the interface-dominated hetero-zone interaction. In this report, we focus on two important issues to reveal the mechanisms of hetero-zone interaction in herterostructured materials: (1) How does strain develop in different domains? (2) What happened at interface of hetero-zones and how does interface affect the development of internal stress and work-hardening? Heterogeneous laminate and gradient materials were used to study these issue. Two typical deformation phenomena, dispersed stable strain bands and interface-affected zone, were experimentally detected and the mechanisms of hetero-zone interaction on the strain accommodation/delocalization were discussed based on micro-mechanics at interface. Our studies provide new insights into the deformation and load-bearing mechanisms of herterostructured materials.

Jacob Huang

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Quantifying the hetero-deformation induced strengthening in bimodal grain structure

The strengthening and toughening by heterogeneous microstructures in multi-principle element alloys have been received attention lately. In some cases together with grain size strengthening and precipitation hardening, the tensile strength can be upgraded to 1.5-2.3 GPa, still with elongation about 15%. In this study, a single-phase bimodal grain structure is under consideration to develop a physical model to quantify hetero-deformation induced (HDI) strengthening at the yield point, which cannot be simply predicted by conventional rule of mixture. Based on the classic theory of single-ended continuum dislocation pileup, the modified model can give solutions to the effective length of interface affected zone (IAZ) as well as the contribution of HDI stress to the overall yield stress. To verify the current model equations, an equimolar CoCrNi single solid solution alloy is selected as a verifying material for experimental testing. The heterogeneous grain structure (HGS) is introduced via a suitable thermal-mechanical treatment, and statistical analysis of microstructure is performed by means of electron backscatter diffraction (EBSD). Our model is found to be capable to predict a yield stress similar to the experimental tensile yield stress value. The reasonable fitting results can not only demonstrate the feasibility of the current modified model, but can also bring the physical explanations for the extra strengthening in materials with HGS.

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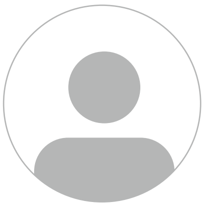
Heterostructured metallic materials: multiscale and multidimensional characterization and tailoring of the microstructure and properties

Heterostructured metallic materials are a new class of materials that exhibit characteristic heterogeneities in structure but significant enhancement in macroscopic properties. The structural heterogeneities are often manifested in the spatial distribution of structural parameters such as morphology, size, shape, phase constituent, substructure, chemical composition, and crystallographic texture. The enhanced properties include strength, ductility, toughness, fatigue resistance, corrosion resistance, and thermal stability. A typical example is overcoming the strength-ductility trade-off dilemma, which has been reported in several heterostructured metals and alloys with structural scales down to nanometers. The local structural heterogeneities and their responses to external loading are the keys to understanding the overall behaviors of the heterostructured materials. Multiscale and multidimensional characterization of the microstructure and mechanical behavior has been carried out in different material systems to analyze the evolution of local variations in structure and stress to understand the underlying mechanisms responsible for enhancing macroscopic properties. However, many fundamental issues concerning the structure-property relationships have not been well understood. In this presentation, examples are shown to demonstrate the recent progress in the multiscale and multidimensional characterization of the structural and property heterogeneities and to discuss its role in understanding the fundamental mechanisms contributing to the enhancement of the macroscopic properties.



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Gradient bulk nanostructures with exceptional strength

Plowing of tailored wedge shaped micro-asperities along the surface of Cu induces steep gradients with increasing subsurface depth that include size scales from 3.5 nm to 150,000 nm with a high hardness of 3.4 GPa at the finest scale. A steep gradient in the deformation microstructure size scale that coarsens with increasing depth is measured with transmission electron microscopy and includes a high dislocation density in between the medium to high angle boundaries. Microprobe and STEM (scanning transmission electron microscopy) show that the nanoscale structure is stabilized by Fe. Iron is transported by dislocations deep into the Cu subsurface by extreme strains. Subsurface stresses are calculated based on the measured structural parameters in a linear addition of the Hall-Petch formulation for the inverse spacing of geometrically necessary boundaries, $\sqrt{1/D_{\alpha v}^{GNB}}$ plus Taylor dislocation hardening, $\sqrt{\rho_{\alpha v}}$. A further unification of these parameters is made since the density $\rho_{\alpha v}$ is directly proportional to $1/D_{\alpha v}^{GNB}$. A quantitative energy balance between the friction and deformation energies corroborate the high hardness and extended stress-strain data for application to hard components and metal processing.

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Schwarz crystal in metals

Grain boundaries with more open structures and excess energies are less stable compared with the close-packed crystalline grains, especially in nanograined metals with a very high density of grain boundaries. When the grains are small enough, the unstable high-density grain boundaries were thought to transform into metastable amorphous states, as evidenced in some alloys. Recently, we discovered a new type of metastable state in extremely fine-grained polycrystalline Cu and other metals. As the grain size is reduced to a few nanometers with straining, the grain boundaries evolve into a three-dimensional minimal surface structure constrained by twin boundary networks, which is named as Schwarz crystal structure. The Schwarz crystal structure in Cu remains stable against grain coarsening at temperatures close to the equilibrium melting point and exhibits a high strength close to the theoretical value. In Al-Mg alloy with Schwarz crystal structure, atomic-diffusion-controlled second phase precipitation, grain coarsening and even melting processes are suppressed significantly. The apparent across-boundary diffusivity was reduced by about seven orders of magnitude at temperatures near the equilibrium melting temperature.

Gang Liu

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Freezing solute atoms in nanograined aluminum alloys via high-density vacancies

Low-temperature decomposition of supersaturated solid solution into unfavorable intergranular precipitates is a long-standing bottleneck limiting the practical applications of nanograined aluminum alloys that are prepared by severe plastic deformation. Minimizing the vacancy concentration is generally regarded as an effective approach in suppressing the decomposition process. Here we report a counterintuitive strategy to stabilize supersaturated solid solution in nanograined Al-Cu alloys via high-density vacancies in combination with Sc microalloying. By generating a two orders of magnitude higher concentration of vacancies bonded in strong (Cu, Sc, vacancy)-rich atomic complexes, an excellent thermal stability is achieved in an Al-Cu-Sc alloy that precipitation is completely suppressed up to ~ 230ºC. The solute-vacancy complexes also enable the nanograined Al-Cu alloys with unexpectedly higher strength, greater strain hardening capability and ductility. These findings provide new perspectives towards the great potentials of solute-vacancy interaction and the development of nanograined alloys with high stability and excellent mechanical properties.

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Synthesis and nanoscale heterogeneity mapping of amorphous/crystalline laminated metals

In this work we report the novel synthesis of novel heterogenous bulk metallic glass (BMG) – metal nanolaminates via accumulative roll bonding. Zr-based BMGs are bonded with Ni via multipass rolling at temperatures within the supercooled liquid region of the BMG. Microhardess is used to probe the thermos-mechanical history on microstructural evolution. Scanning Nano-structure electron microscopy (SNEM) was used to understand the complex chemical nature of the microstructure at the BMG/Ni interfaces. More specifically, scanning electron diffraction (also known as 4D-STEM) coupled with electron atomic pair distribution function analysis (ePDF) is used to understand the local order (structure and chemistry) as a function of position in our complex multicomponent system. We show the ability to fabricate amorphous/crystalline laminates with interface widths or 3-4 nm, and present a new approach to probe understand the chemical and structural homogeneity within those regions, thus revealing critical insights into nanoscale heterogeneity formation mechanisms and nanoscale features that control the bulk mechanical response and other properties.

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On the structural origins of novel properties of some heterostructured materials

Interactions and competitions among different components in heterostructured materials (HSMs) lead to many intriguing and unprecedented properties. However, elucidating the structure-property relationship in HSMs is a challenging task due to their complex structures. We have been utilizing advanced synchrotron X-ray and neutron techniques in combination with other methods to unravel the structural origins of novel properties of some HSMs. In this talk, we will present an in-situ synchrotron high-energy XRD study of a NiTi/Nb nanocomposite, which exhibit large elastic strain, low modulus and high strength [Hao et al., Science, 339, 1191 (2013)]. The results show that the superior mechanic property is due to a strong coupling between Nb nanowires and the NiTi matrix. We will also show a recent finding of supercritical elasticity in NiCoFeGa multicomponent alloys, which exhibit over 15% non-hysteretic elasticity, a small temperature dependence, high-energy-storage capacity and ultra-stable cyclability. In-situ synchrotron X-ray diffraction measurements show that the supercritical elasticity is correlated with a stress-induced continuous variation of lattice parameters accompanied by structural fluctuation. Neutron diffraction and electron microscopy observations reveals an unprecedented microstructure consisting of atomic-level entanglement of ordered and disordered crystal structures, which can be manipulated to tune the supercritical elasticity [Chen et al., Nature Materials, 19, 712 (2020)]. The discovery of this type of large elasticity related to the entangled structure paves the way for exploiting elastic strain engineering and development of related functional materials.

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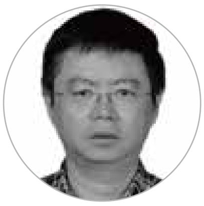
The effects of interface and plastic strain gradient in heterostructured metals

It remains a challenge to understand the micromechanics near the interface and the corresponding effects on stress-strain behavior. In the deformation of heterostructure, interface affected zone (IAZ), characterized by high strain gradient concentration in a constant characteristic width of a few micrometers, is formed to coordinate inter-zone deformation heterogeneity. Along with the accumulation of geometrically necessary dislocations, back stress and forest hardening develop in IAZ and produce extra work hardening response. Simulations reveal that the extra work hardening increases proportionally with IAZ volume fraction, and the best strength-ductility combination is reached as IAZ approaches saturation. In addition, IAZ unifies the effects of zone configuration, mechanical incompatibility and zone volume fraction. Therefore, IAZ may be considered as a unified key microstructural factor that controls the synergistic work hardening of heterostructures. These findings point out the mechanical essence of heterostructure design: building high-density interface to popularize strong strain gradient effects throughout the material. More future work should probably focus on the microstructure design of interface to improve IAZ effects.



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Engineering ordered heterostructured materials with ultrahigh energy density

Heterostructured materials (HSMs) with a random or ordered arrangement of structural constituents have the potential to create enhanced properties or transformative functionalities, as they provide an effective way of engineering inhomogeneous structures to overcome the conflicting material characteristics, such as strength and ductility. As an emerging field, the mechanical properties of HSMs have been intensively studied, but the functional properties of HSMs still remain unexplored. In this talk, we use permanent-magnet materials as an example to demonstrate the efficacy of heterostructures to enhance the properties of functional materials. We focus on the design of HSMs with an ordered arrangement of structural constituents. Such ordered HSMs enable us to achieve previously inaccessible new magnetization reversal mechanisms and/or enhanced magnetic properties.

First, we describe the fabrication of bulk hybrid nanomaterials comprising soft and hard-magnetic components with well controlled individual component characteristics, including grain size, distribution, content, and crystal orientation. This achievement has been realized through devising new processing principles and technologies, with a combination of top-down and bottom-up approaches. Then, we report how to build a bulk hybrid nanostructure with an ordered arrangement of constituent components, including gradient structure, layered structure, and core/shell structure. The resulting gradient and layered ordered nanostructures exhibit a record-high energy density for isotropic and anisotropic bulk permanent-magnet materials with less rare-earth metals, respectively. The excellent properties are achieved by creating new magnetization reversal mechanisms in the ordered structures, which are inaccessible with both the homogeneous structures and the disordered inhomogeneous structures. These findings open up new opportunities for fabricating high-performance permanent-magnet materials with reduced rare-earth metals and for engineering next-generation ultrastrong permanent magnets by constructing ordered HSMs. We anticipate that other functional properties beyond magnetism, such as the thermoelectric, ferroelectric, and catalytic properties, could also be enhanced by designing HSMs with atomic-scale, nano-scale, and/or micro-scale ordering.

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Dislocation mechanisms of HDI hardening in heterostructured materials

Different from the conventional uniform materials, heterostructured material contains both soft and hard zones in micro-scale. To coordinate the deformation incompatibility, huge hetero-deformation induced (HDI) strain hardening occurs during plastic deformation. As a result, heterostructured materials usually have outstanding ductility even under a very high level of flow stress. The HDI stress consists of a back stress in the soft zone and a forward stress in the hard zone. Understanding their physical mechanism is helpful for developing novel heterstructured materials.

In this work, the real-time evolution of dislocations as well as their interaction with hetero-interfaces are investigated by in-situ TEM characterization. We clarify two important mechanisms. First, dynamic Frank-Read dislocation sources are found in the coarse grains (the soft zone) to emit geometric necessary dislocations, leading to a strain gradient near the interface. Meanwhile, a long-range back stress is generated due to the piling-up of GNDs. Second, interfacial dislocation sources are formed in the ultra-fine grains (the hard zone), which continuously emit dislocations with same Burgers vector, resulting in tilting of the ultra-fine grains.

In addition, we find that interfacial dislocation sources are dominated in multi-principle alloys (HEA). Most of the dislocations are emitted from grain boundaries or other interfaces, forming unique planar arrays in slip bands. In order to increase the piled-up GNDs, the dislocation will continuously reflect from the hetero-interface to help increasing of HDI strain hardening. The cross-slip of full screw dislocation is the mechanism for the dislocation reflection.

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Deformation behaviors of layered metallic materials revisited from local stress and local strain

Synchronous enhancement of strength and ductility is one of the eternal topics in the community of metallic materials. Such a strength-ductility trade-off dilemma has been evaded in recent years, e.g., within heterostructured materials, multiphase materials, high entropy alloys etc. A series of physical mechanisms were thus proposed including back-stress strengthening, strain gradient, multiple interface effect, lattice distortion effect, etc. The present project focuses on the ‘local stress’, which is the source of plastic flow and the “local” represents the affected scale of the ‘stress’. A local-stress/strain-regulated mechanism is then developed to rationalize the fundamentals of the synergy between strength and ductility. Specifically, the layered metallic materials are selected as model materials, and analyzed by an integrated technology enabling the local stress characterization from atomic- to macro-scales based on electron microscopies and synchrotron radiation and neutron scattering. Several of key deformed sub-structures such as dislocation configurations, twins, slip bands, shear bands are characterized and correlated with the evolution of local stress upon loading. Based on these findings, the local-stress/strain-dependent regulation criterion for strength-ductility synergy of metallic materials is presented, which further guides the development of high-performance metallic materials.

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In-situ investigation of local plastic deformation in aluminum with near-micrometer grain size and heterogeneous grain-size distribution and arrangement

By control of the sintering conditions and powder characteristics is it possible to prepare microstructures in a fully recrystallized state with controlled grain size using spark plasma sintering. This has been used to investigate plastic deformation and mechanical properties in the near-micrometer grain-size regime in aluminum of samples with heterogeneous grain-size distribution and arrangement, by control of powder size and mixing conditions. Both electron backscatter diffraction and digital image correlation have been used during in-situ loading of tensile samples in a scanning electron microscope, providing complimentary information on spatial variations in local crystal rotations and the local plastic deformation. In the case of a sample with a mixture of fine and coarse size grains, the plastic deformation takes place preferentially in the larger grains, but only to a limited extent, whereas in macroscopically layered samples deformation is dominated by strain localization in the fine grain layers. These studies have been supplemented by in-situ loading using high brightness synchrotron radiation to investigate heterogeneity of plastic yielding in the elastic-plastic transition region.

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Heterogenous nanostructured in nanotwinned inconel alloys

Nanotwinned (NT) alloys were synthesized via magnetron sputtering and subjected to an aging treatment that ultimately induced a transformation from a highly NT structure to a heterogeneous nanostructured material with a unique and complex gradient grain topology. The heterogeneous microstructure contains domains consisting of columnar NTs, nano-grains, and abnormally large grains with diameters greater than 1 µm, which represents a material with a wide range of grain sizes and morphologies. In this presentation, the microstructure of three distinct domains with variable grain size, precipitate formation, and morphologies will be discussed. These include: a NT region, a nanocrystalline structure and an abnormal recrystallization region where rafted structures, M23C6 and δ precipitates were observed. The effect of strain on the microstructural evolution will be highlighted as a route to expand the current design space for heterogeneous microstructures.

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Industrial manufacturing of Heterogeneous Materials: Preliminary investigation and perspectives

The progress of industrial processing of heterogeneous TA1 (GR1) by Ansteel Beijing Institute is reported. Low-iron-and-oxygen heterogeneous TA1 rods with ϕ30~60 mm and UTS of 600~700 MPa were successfully prepared by conventional forging process. The room temperature and high temperature performance evaluation and microstructure evolution analysis were carried out on the heterogeneous TA1 rods. The problems that may be encountered in the industrialization of heterogeneous materials are discussed, and relevant suggestions are put forward.

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Understanding the role of heterostructured phase boundaries in copper-based lamellar metallic composites

Heterostructured materials (HSM) are a new class of materials that provide an extraordinary high potential for improving materials properties far above what is known for currently used engineering materials. As for conventional materials it is also essential for HSM to be able to link particular micro-/heterostructural features to the corresponding material properties and their influences upon. This is not easy in monolithic materials, and gets even more complex for HSM, where the microstructural aspects are then paired with further "architectural (geometrical)", chemical and physical influences. At the interfaces of HSM the different properties of the heterogeneous constituents are enforced to anyhow match to each other in order to keep the overall materials compatibility. Thus, beside the microstructural influences on the mechanical properties of a single constituent, the additional effects of heterostructured interfaces to the mechanical behavior are of high relevance. Recent research shows that especially phase boundaries play an important role for the overall material properties. To tackle this question a well-defined and highly ordered structure is necessary to separate the influence of phase boundaries on material properties from other effects. Lamellar metallic composites (LMCs), which can easily be produced by accumulative roll bonding (ARB), fulfill these requirements. The individual layer thicknesses and corresponding number of interfaces can be easily designed to cover the whole thickness area from several hundreds of micrometer (few phase boundaries) down to several nanometers (many phase boundaries), which gives the opportunity to analyze basically the same heterostructured layered material on different length scales and different constituents.

In this work we varied the constituent's volume fraction and layer thickness of copper-based LMCs (Cu/Nb, partially Cu/Fe by ARB) systematically. Microstructural analysis using SEM and TEM microscopy reveal a continuous layered structure in all LMCs while the mechanical properties show a distinct difference between low cycled sheets (less phase boundaries, thick layers) and highly cycled sheets (high amount of phase boundaries, thin layers). Mechanical testing like tensile, nanoindentation or conductivity tests were performed and correlated with the corresponding microstructure revealing the importance of a in depth understanding of the contribution of heterostructured interfaces to the overall material properties.

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Plasticity in Laser Processed Al-Si Eutectic Alloys

A range of heterogeneous Al-Si microstructures, comprising of nanoscale Al-Si eutectic domains with nanotwinned Si fibers and sub-micron-scale primary Al, with or without Si nano-precipitates, were fabricated by processing as-cast Al-20wt.%Si alloy using laser rapid solidification. In situ tensile testing in a scanning electron microscope demonstrated high tensile strength, ≈600 MPa, and ductility, ≈10%, and high strain hardening rate, ≈7 GPa. Microstructural characterization revealed the plastic co-deformation mechanisms between soft Al grains and the surrounding relatively harder nanoscale Al-Si eutectic. The progression of plasticity in nanoscale Al-Si eutectic with increasing applied strain is accommodated by dislocation plasticity in the nano-Al channels and cracking in Si nanofibers. The propagation of nano-cracks is suppressed by surrounding Al, retaining good ductility of the sample. Cross-sectional scanning/transmission electron microscopy of nanoindents revealed a transition in morphology from high aspect ratio nano-fibrous Si to short nano-fibrous Si, preferentially located along triple junctions of the dynamically recovered sub-grains in Al. Molecular dynamics simulations of the interaction of glide dislocations in Al with the flat Si/Al interfaces revealed climb and cross-slip mechanisms but no direct slip transmission into Si. The role of the heterogeneous Al–Si microstructure in enhancing strain hardening rate and resulting in plasticity in micro-tensile sample even after fracture of nanoscale Si fibers is discussed.

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Thermally and mechanically induced hererogenity in high-entropy alloy: short – range order

Short-range order (SRO) would belong to ultrafine-scaled heterogeneity. Herein, we report two different SRO types in an Fe40Mn40Cr10Co10 (at%) high-entropy alloy. One is thermally activated chemical SRO that emerges with specific heat-treatments, and the other is displacive SRO that emanates from tensile deformation at liquid-N2 temperature. The degree/extent of the former one are tailored by altering annealing temperatures, while by tuning loading rates for the latter one. Atomistic Monte Carlo simulations predicted that 'preference for unlike pairs and avoidance of like pairs' and 'preference for Cr–Cr like pairs' in the first neighboring shell were introduced by lowering the temperatures of the system. Besides, scanning and high-resolution transmission electron microscopy together with diffraction patterns revealed not only the microstructural features responsible for the strain-induced SRO but also the dependence of the ordering degree/extent on the applied strain rates. These experimental findings were consistently supported by molecular dynamics simulations and associated diffraction patterns, i.e., mechanically derived SRO generated the diffuse discs or spot-like scattering at the ½{311} locations in the reciprocal-space electron diffraction patterns along the $[1\bar{1}2]$ zone axis. Further, the mechanical response and multi-length-scale characterization pointed to the negligible impact of strain-induced SRO on yield strength, mechanical twinning, and martensitic transformation. Owing to these features, we regarded the localized SRO as mechanically derived SRO rather than diffusion-mediated chemical SRO that would be destroyed by planar dislocations during deformation. Lastly, we outline here that while the chemical SRO-related heterogeneity shows 'deformation-induced SRO-to-disorder transition', the mechanically derived SRO heterogeneity exhibits 'strain-induced disorder-to-SRO transition'. We hope that the current study provides important insights into the mechanical properties of many heterostructured alloys that are prone to either disorder-to-order or order-to-disorder transition at the short rages.

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Heterostructure induced strain delocalization by forming dispersed strain bands

Trans-scale digital image correlation reveals that the uniform elongation of heterostructures is largely accommodated by forming dense, dispersed and stable strain bands (SBs). Dispersed SBs were nucleated from the elastic-plastic transition stage, reached density saturation at the low-strain stage, and remained arrested by the ductile zone. The limited strain hardening capability of nanostructured zone is a prerequisite for nucleating SBs, and the synergistic inter-zone constraint is the necessary condition for the dispersive nucleation and stable evolution. The change of stress state in strain banding region enables the activation of additional plastic mechanisms, which helps to retain work hardening. Dispersed strain bands modify the strain path of constituent zones and consequently the behavior of heterostructure. The remaining issues of dispersed SBs lie in the crystallographic nucleation mechanism, the physics behind SBs-zone boundary interaction, and the derived principle for optimizing microstructure design.

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Creating compositional and structural heterogeneities for controlled strain release during deformation

Shear deformation in materials, including dislocation glide, mechanical twinning and martensitic transformations in crystalline solids, and shear banding in metallic glasses, share key common features such as autocatalysis by long-range elastic interactions and strain avalanche. To achieve desired stress-strain behaviors for a given application, microstructures need to be tailored judiciously to have precisely controlled strain release during both superelastic and plastic deformations. In this presentation, we review some novel microstructure design strategies to regulate strain release during shear deformation. In particular, using a combination of theoretical modeling, computer simulation, and experimental testing and characterization, we demonstrate that fine scale concentration modulations created by different means are highly effective in converting strongly firstorder, sharp martensitic transformations into apparently continuous transformations, offering linear superelasticity with nearly zero hysteresis, ultralow modulus, and Invar and Elinvar anomalies. Fine-scale phase stability modulations accompanying concentration modulations can also conduce to a fine dual-phase microstructure that offers high strength and prolonged TRIP effect for high work-hardenability and large uniform elongation. We then demonstrate that deformation twins in austenite can harbor martensitic embryos because of the intrinsic coupling between deformation twinning and martensitic transformation. Thus, a high density of deformation twins in austenite also offers nearly linear superelasticity with ultralow modulus and slim hysteresis. Finally, we show some examples on the design of gradient and hierarchical precipitate microstructures intended for regulating dislocation plasticity for a synergistic combination of strength and ductility. These new design strategies could allow us to achieve unprecedented stress-strain behavior in both structural and functional materials.

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Characterize microstructures of heterostructured high-entropy alloys via correlative EBSD and ECCI

We investigate the microstructure and deformation substructure evolution in heterostructured high-entropy alloys (HEAs) by means of a scanning electron microscopy (SEM)-based approach, which involves correlative electron channeling contrast imaging (ECCI) and electron backscatter diffraction (EBSD) techniques. The combinational use of EBSD and ECCI reveals microstructure of the additively manufactured HEAs across various length scales, including a bimodal grain structure, low angle boundaries, and dislocation networks, along with the quantitative evolution of geometrically necessary dislocations (GNDs) distribution. The deformation microstructure evolution of the HEA upon loading is uncovered to clarify the strain hardening mechanism. The present approach shows comparable resolution to traditional bright field transmission electron microscopy (TEM) imaging, yet with far higher efficiency and affordability.

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Achieving high strength and large elongation in steels via heterogeneous structure design

Steel is the most widely used structural material. Improving the strength of steel is one of the important directions for the carbon neutrality of the steel industry and the whole society. However, a good elongation is required to ensure good formability for high-strength steel used in various areas, i.e. car body and corrosion resistance pipe. A synergy of strength and elongation is highly desired for advanced steel. In this presentation, three approaches are shown to obtain steels with high strengths and large elongations via heterogeneous structure design. I) Heterogeneous grain structure: interstitial-free steel with a deformed-and-recrystallized lamellar structure was prepared by alternative stacking initially fully annealed plates and cold-rolled plates, cold forging and annealing; II) Heterogeneous phase structure: 0.1C5Mn3Al steel with a ferrite-and-martensite lamellar structure was prepared by hot-rolling at an intercritical temperature; III) Heterogeneous phase+grain structure: a duplex stainless steel with recrystallized ferrite lamellae and fine recovered austenite lamellae was prepared by cold rolling and annealing at a high temperature for a short time. The microstructural evolutions and mechanical behaviors of these three steels were studied; and the effects of back-stress and interface accommodation on the mechanical properties were discussed.

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Mechanical properties and deformation mechanisms in high entropy alloys with dual heterogeneous/graded structures

High entropy alloys and medium entropy alloys have attracted extensive research interests recently due to their superior mechanical properties and unique deformation mechanisms. In the present study, dual heterogeneous/graded structures (both grain size and volume fraction of precipitate) have been designed and fabricated in one high entropy alloy and one medium entropy alloy, and the tensile properties and the dynamic shear properties have been investigated. The corresponding deformation mechanisms have been revealed by detailed microstructure characterizations. Dual heterogeneous/graded structures were found to have better synergy of strength and ductility under both quasi-static conditions and impact dynamic conditions, as compared to single heterogeneous/graded structures. More severe strain gradients and higher density of geometrically necessary dislocations were observed to be produced at various domain boundaries in the dual heterogeneous/graded structures, resulting in stronger hetero-deformation-induced extra hardening for better mechanical properties, as compared to single heterogeneous/graded structures. Shearing and bowing hardening mechanisms were observed for L12 and B2 precipitates, respectively. Higher volume fractions of B2 and L12 phases at the topmost layer induce stronger precipitation hardening, which compensates the diminished strain hardening due to the reduced grain size at the topmost layer for better tensile ductility in the structures with combined gradients. The observed strength has been discussed based on dislocation strengthening, grain boundary strengthening, Orowan-type bowing strengthening of B2 nano-particles, shearing strengthening of L12 nano-particles, strengthening of chemical short-range order and hetero-deformation-induced strengthening. Phase transformations from FCC phase to B2/σ phase were observed under impact dynamic conditions, which were never observed under quasi-static conditions for the same alloys. These newly observed phase transformations can be attributed to high strain rate, high strain/stress magnitude, high adiabatic temperature rise and fast-cooling process within adiabatic shear bands. The present findings should provide insights for tailoring microstructures for achieving superior mechanical properties and for applications of high entropy alloys or medium entropy alloys with heterogeneous structures under extreme impact conditions.

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The nature and roles of heterogeneous structures in sustaining high strength-ductility synergy in PM titanium and titanium alloys

By using different powder metallurgy routes involving hydrogenation and dehydrogenation of titanium, powder processing and thermomechanical powder consolidaiton, together with heat treatments, commercially pure titanium and near α and α+β titanium alloys such as Ti-2Al-1.3V (wt%), Ti−3Al−2Zr−2Mo, Ti−6Al−2Sn−4Zr−2Mo and Ti-4Al-4Mo-4Sn-0.5Si alloys with heterogeneous structures are fabricated. When being optimized, the heterogeneous structures render the alloys with both high strength and excellent tensile ductility. This report is to present the findings from the investigation into the microstructures, tensile properties and fracture behavior of PM CP titanium and titanium alloys with heterogeneous structures, and discuss the underlying reasons and mechanisms of the high strength-ductility synergy sustained by the composition and microstructures. There are also cases where heterogeneous structures cause unfavorable mechanical properties such as high strength and poor ductility or relatively low strength and low ductility. Such cases are also presented and discussed.

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Ultrahard twinned substructure induced by martensitic transformation in steels

Twinned substructure represents a category of martensite containing more alloy elements in particular carbon, namely twinned martensite. However, even though the twinned substructure is of nanometer-scale, it is believed to be an insignificant contribution to the hardening. Besides, the twinned substructure is well accepted having the origin from the {112} deformation twinning that was thought to accommodate the shape strain during the martensitic transformation. Consequently, twinned substructure is unlikely for the typical lath martensite that was formed in low carbon and low alloy steels, where dislocation slip accommodates the shape strain. Here we report our recent investigations on the martensite induced in pure iron, IF steel, FeCr, low-, medium- and high-carbon steels. The following findings were highlighted: 1) the twinned substructure has the origin related to the orientation relationship between martensite and austenite rather than the {112} deformation twinning; 2) Nanotwinned substructure can give rise to ultrahigh hardness; 3) the hardening can be independent of carbon content.

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Mechanical behavior of nanostructured metallic materials with thick grain boundaries

Grain refinement has been extensively used to strengthen metallic materials for decades. Grain boundaries (GBs) act as effective barriers to the transmission of dislocations and consequently lead to strengthening. Conventional GBs have a thickness of 1-2 atomic layers, typically 0.5 nm for most metallic materials. However, when GB thickness increases to several nm, the mechanical behavior of metallic materials can be drastically altered. Here we show an example of thick GBs in nanocrystalline Ni alloy produced by severe plastic deformation. In-situ micropillar compression studies coupled with MD simulations suggest that the thick GBs are strong barriers to the transmission of dislocations. In another example we show that nanocrystalline CoAl with thick GBs exhibits ultra-high yield strength and significant compressive plasticity. Transmission electron microscopy and MD simulations reveal that the thick GBs play a pivotal role in tailoring the plasticity of intermetallics. The implications of these findings on the design of advanced materials will be discussed.

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Atomistic analysis of shear band formation in metallic nanolayered composites

Metallic nanolayered composites (MNCs) are a special class of composite materials made from alternative layers of different metallic constituents with the layer thickness at nanometer length scales. They have gained considerable interests in recent years due to their distinctive structures, enhanced strength, high wear resistance, and improved radiation damage tolerance. Mechanical testing results showed that MNCs exhibited 5-10 times higher strengths than their single-phase counterparts and a clear size effect of increasing strength with decreasing the layer thickness. However, the shear band (SB) formation under compression or early fracture under tension limits their potential applications. In this work, we explore the effect of the layer thickness and crystal structures on the shear localization and shear band formation in FCC/FCC and FCC/BCC MNCs with flat interfaces via molecular dynamics simulations. We analyze the configuration of dislocation structures, von Mises shear strain distributions and the change in the separation distance of nearest neighbor atoms in the deformed samples with various layer thicknesses. Our simulation results achieve good agreement with previous experimental results, and demonstrate that the strain softening observed in samples with small layer thickness is triggered by the shear localization. The analysis revealed the shear band formation in MNCs does not depend on the layer thickness and crystal structures, but also the stacking fault energy of each phase. Our work uncovered the origin of the SB formation in MNCs with flat interfaces and can shed light on the design of MNCs with superior mechanical properties.

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Strain hardening behavior and microstructure evolution of gradient-structured Cu-Al alloys with low stack fault energy

The "trade-off" between strength and ductility are important topics in structural materials research. Heterostructured materials are an emerging class of materials with superior performances because of their outstanding work hardening capability. In this work, a type of heterostructured material, a gradient structured Cu-Al alloy, was produced by surface mechanical attrition treatment (SMAT) at liquid nitrogen temperature. Microstructure observation and stress relaxation test were used to study the deformation mechanism of this material. The effect of stacking fault energy (SFE) on the mechanical behavior and deformation mechanism of materials has been preliminarily explored in this study. Shown as the research, after SMAT processing, the yield strength was increased to more than 1.5 times, and the ductility remained almost unchanged. In conjunction with hetero-deformation induced (HDI) hardening, stacking fault energy is another important factor to increase the strain hardening in the system. Low stacking fault energy increased the density of stacking fault, and led to a finer spacing of nano twins (~5.4 nm) and higher dislocation storage (8 × 1013 m-2) in the SMATed Cu-Al alloy at the intermediate strain stage. A significant up-turn of strain-hardening rate was also induced by low stacking fault energy.

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Strain partitioning enables excellent tensile ductility in precipitated heterogenous high-entropy alloys with gigapascal yield strength

High entropy alloys (HEAs) with grain-scale heterogeneous structure and coherent precipitates have shown gigapascal strength and considerable ductility. However, the origins of the excellent ductility of the HEAs with both precipitates and grain-scale heterogeneous structures are relatively less explored and not well understood. It is also still challenging to obtain such precipitated heterogeneous HEAs through efficient and economical thermomechanical processing procedures. Here, through single-step heat treatment, we developed a $Ni_2CoCrFeTi_{0.24}Al_{0.2}$ HEA with an excellent yield strength of ~1.3 GPa and tensile elongation of ~20%. Using multiple length-scale microstructure characterizations and micro-digital image correlation analysis, we revealed the strengthening and toughening mechanisms of the novel HEA. Our results showed that the grain-scale heterogeneous structure with $L1_2$ precipitates ranging from ~10 – 100 nm is responsible for the excellent strength-ductility combination. The good ductility is attributed to the strain-partitioning-induced additional deformation modes, i.e., deformation twinning and microbands, as well as the efficient hetero-deformation induced strain hardening effect. The superior yield strength is mainly due to the effective combination of precipitation hardening and dislocation strengthening. These findings not only provide a facile route to develop strong and ductile alloys but also deepen the understanding of the deformation mechanism of hetero-structured materials.

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Microstructural features in bimodal structure-property linkage

A recent research direction for microstructural design is to overcome the strength-ductility trade-off by introducing heterogeneous structures, such as bimodal, gradient, or lamellar structures. Many experimental studies have revealed that additional strengthening is caused by differences in deformation mechanism between soft and hard domains of heterogeneous materials. The soft domain undergoes plastic deformation prior to the hard domain, which leads to the generation of geometrically necessary dislocations (GNDs) inside the soft domain near an interface with the hard domain. These GNDs are assumed to be primarily produced by Frank-Read dislocation sources; then, they would pile up at the interfaces, giving rise to heterogeneous-deformed-induced (HDI) strengthening. As a heterogeneous structure, the bimodal structure consisting of fine grains (hard domains) and coarse grains (soft domains) can be related to mechanical properties by considering the heterogeneous deformation mechanism. In this presentation, the effects of their grain sizes, volume fractions, and spatial distribution within a representative volume element (RVE) are investigated to explore bimodal structure-property (SP) quantitative linkages employing a microstructure based-finite element modeling (FEM) simulation. The developed dislocation-based constitutive model assumes GNDs are generated at the interface between soft coarse grain (CG) and hard fine grain (FG) domains on the CG side. Based on this approach, we propose an optimal bimodal structure to maximize synergy in mechanical properties of heterogeneity. This work demonstrates that the bimodal microstructure-property linkage can be analyzed quantitatively to facilitate finding optimal heterogeneous equiaxed bimodal structures.

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Simultaneously enhanced strength and strain hardening capacity in high-entropy alloy via harmonic structure design

In the past decade, many HEAs with various crystal structures have been proposed, among which simple face-centered cubic (FCC) structured HEAs have received the most attention, due to their excellent ductility, superior fracture toughness and high radiation tolerance. However, the strength of FCC-HEAs is insufficient, especially the low yield strength (usually below 350 MPa) at room temperature, which limits their practical applications as advanced structural materials. Therefore, it is quite desirable to develop novel microstructural design strategies to improve the strength and ductility synergy of FCC-HEAs.Harmonic structure (HS), consisting of coarse-grained (CG) areas uniformly embedded in three dimensional continuously connected ultrafine-grained (UFG) areas, is considered as an effective micro-structural design strategy to achieve enhanced strength and ductility in metallic materials.

In the present study, HS designed non-equiatomic FeMnCoCr high-entropy alloy samples with tunable shell fractions (ranging from ~16% to ~70%) were successfully prepared via controlled mechanical milling and subsequent sintering. Microstructure observations suggested that the shell region was composed of fully recrystallized UFGs with a mean grain size below 1 μm. Tensile test revealed that the HS designed samples exhibited simultaneously enhanced strength and strain hardening capability than those of the homogeneous structured counterpart. Particularly, the ultimate tensile strength and uniform elongation of the sample with a shell fraction of ~70% were 1228 MPa and 12.4%, respectively, demonstrating superior strength-ductility synergy. The HS designed samples exhibited simultaneously enhanced strength and strain hardening capability than those of the homogeneous structured counterpart. The significantly enhanced strength was due to the high-volume fraction of the shell region, which was composed of fully recrystallized UFGs. The enhanced strain hardening rate was associated with the unique three-dimensional core-shell structure as well as the activation and interaction of multiple deformation mechanisms.

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Investigations on ballistic impact performance of gradient structured AZ31 Mg alloy with enhanced strength and plasticity

Due to a combination of strength, low density and high specific damping capacity and high shock absorbency, Mg alloys are considered as suitable and prospective armor materials in automobile and aerospace vehicles. The application of lightweight components can effectively reduce the overall weight and hence fuel consumption. Mechanical properties improvements would further promote its ballistic resistance. In our work, the introduction of gradient twinning structures on both sides of a Mg alloy plate can simultaneously enhance its strength and plasticity. Different from common insights on mechanical properties improvements from the multiplication of geometrical necessary dislocations, the strain field measurements and microstructure observations demonstrate that abundant twin-twin interactions due to higher strength and multi-axial stress state in the core region play major roles in increasing the work-hardening capacity, consequently a better combination of strength and plasticity. On this basis, we further investigate its ballistic resistance capacity. Compared with homogeneous Mg alloy plate in the same dimension, the ballistic energy absorption of gradient structured plate is improved by 50%. Meanwhile, the penetration failure modes after impacts for these two materials are different distinctly. In order to clearly interpret the effects of properties enhancement and gradient structure on the ballistic impact performance, we build finite element models to analyze the plastic deformation and penetration failure process, particularly focusing on studying the propagation of stress waves through the gradient structure. The simulation results reveal the lamination crack along the boundary of rear gradient layer and a columnar plunger cylinder after penetration failure, whereas for the homogeneous plate the rear surface exhibits evident tension failure due to the reflection of stress wave and a pyramidal plunger is generated. Moreover, with an increasing strength adiabatic shear localization becomes one of main reasons for causing the cylindrical plunger failure in gradient structured Mg alloy. Microstructure observations and fracture morphology have demonstrated the appearance of adiabatic shear bands near the columnar boundary. Therefore, the failure mechanism transition causing by gradient structure design should be responsible for the improved ballistic resistance. Such a strategy may provide a new path for producing advanced materials in armor protection structures.

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Manipulation of gradient structure profile in a CrMnFeCoNi high-entropy alloy for superior mechanical properties

We explore how different gradient structures of an equiatomic CrMnFeCoNi high-entropy alloy affect its mechanical properties. The alloy was processed using the rotationally accelerated shot peening technique. Varying processing parameters leads to different gradient hierarchical structures that subsequently change the mechanical behaviour of the material. Microstructures along the depth from sample surface were characterized using advanced electron microscopy. Mechanical properties were obtained using microindentation and uniaxial tensile testing. The quantitative contributions of different structural features including deformation twins and dislocations to the surface hardening were carefully investigated. Based on our study, an appropriate gradient structure profile is recommended for excellent combination of strength and ductility.

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Gradient structured high entropy alloy with improved synergy of strength and ductility: experiments and crystal plasticity simulations

The interstitial high entropy alloy (iHEA) $Fe_{49.5}Mn_{30}Co_{10}Cr_{10}C_{0.5}$ (at. %) with multiple strengthening and plastic mechanisms has proved to achieve a combination of strength and ductility. In this work, gradient structures are successfully produced in the iHEA by using surface mechanical attrition treatment (SMAT). Uniaxial tensile tests, microscopic characterizations, and crystal plasticity modeling are conducted for the gradient structured (GS) iHEAs prepared by different-time SMAT. After 15 mins SMAT, the yield stress of iHEA increases by ~32.6% with almost no reduction in ductility. Although the further increase of SMAT time leads to the loss of ductility, the ultimate stress of GS iHEA after 60 mins SMAT is close to 1 GPa, while the uniform elongation exceeds 10%. The improved strength-ductility synergy benefits from the gradient distributions of grain size, dislocation density and martensite fraction. The ductility loss may be due to the strain localization and grain boundary crack caused by the generation of martensite. Moreover, a size-dependent crystal plasticity model considering multiple plastic deformation mechanisms is developed for the iHEA, including dislocation slip, deformation twinning and martensitic transformation in austenite, as well as dislocation slip and cross slip in martensite. The slip resistance considers the effects of solid solution strengthening, precipitation strengthening, back stress, etc. The simulated results of the iHEAs with different grain sizes fits the experimental results well, verifying the validity of the developed model. Using the isostrain homogenization scheme, the deformation response of GS iHEA in the macroscopic scale can be simulated. It can be analyzed that the initial nanograins, high-density dislocations and high-fraction martensite cause the weak strain hardening ability of the top surface layer, which is supposed to be the intrinsic reason for the surface strain localization after long-time SMAT. Finally, the simulations quantified the contributions of different gradient microstructures to the strength and ductility. This work provides guidance for optimizing the HEA's mechanical properties by microstructural design.

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High-entropy alloy microlattice metamaterials

Mechanical metamaterials such as microlattices are man-made materials that can harness the benefits of architecture through their engineered three-dimensional (3D) geometries and unique structural designs. This talk focuses on how these microlattices are combined with micro/nanoscale size effects and high/medium-entropy alloys (HEA/MEA) to produce metamaterials with superior and tunable mechanical properties, providing an insight on overcoming traditional material property trade-offs, such as strength-ductility, which has limited our structural material selection for many years. An overall perspective on how these HEA/MEA microlattice metamaterials can be designed, manufactured, and applied for a multitude of future engineering applications will be discussed as well.

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The role of pre-existing heterogeneities in copper under shock

There has been a challenge for many decades to understand how heterogeneities influence the behavior of materials under shock loading. Experimental, analytical, and computational techniques have matured to the point where systematic studies of materials under shock loading with complex microstructures are feasible. As interest in complex materials grows, understanding and predicting the role of heterogeneities in determining the dynamic behavior becomes crucial. Early computational studies, hydrocodes in particular, historically preclude any irregularities in the form of defects and impurities in the material microstructure for the sake of simplification and to retain the hydrodynamic conservation equations. Contemporary computational methods, notably molecular dynamics, can overcome this limitation by incorporating inhomogeneities. Pre-existing defects are found in most engineering materials, ranging from thermodynamically necessary vacancies, interstitial and dislocation concentrations to microstructural features such as inclusions, second phase particles, voids, grain boundaries, and triple junctions. Systematic characterization of material heterogeneities before and after shock loading, along with direct measurements of Hugoniot elastic limit and spall strength, allow for more generalized theories to be formed. Continuous improvement towards time-resolved, in situ experimental data strengthens the ability to elucidate upon results gathered from simulations and analytical models, thus improving the overall ability to understand and predict how materials behave under shock loading.

The mechanisms responsible for the collapse of helium-filled bubbles during the passage of shock waves in monocrystalline copper are revealed. Both internal pressure (caused by pre-existing helium atoms) and bubble size are varied in molecular dynamics simulations to understand the atomistic scale deformation as they are subjected to shock compression. Both empty and helium filled bubbles serve as dislocation sources, generating intense, localized plastic regions. A generalized model for dislocation emission is proposed, where the inclusion of shear stress generated by the helium bubble increases the critical stress to generate dislocations at the defect surface, demonstrating the change in plastic deformation.

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Gradient-cell-structured high-entropy alloy with exceptional strength and ductility

Most multicomponent high-entropy alloys (HEAs) lose ductility with increasing strength, similar to conventional materials. Here we controllably introduced novel gradient nano-scaled dislocation-cell structures in one stable single-phase face-centered-cubic HEA, which result in enhanced strength without apparently losing ductility. The sample-level structural-gradient induces the progressive formation of a high density of tiny stacking-faults (SFs) and twins upon early straining, nucleating from abundant low-angle dislocation cells. Furthermore, the SF-induced plasticity and the resultant refined structures, coupled with intensively accumulated dislocations, contribute to the plasticity, extra strengthening and work hardening. Our findings offer a promising paradigm for tailoring properties with gradient-dislocation cells at the nanoscale and advance our fundamental understanding of the intrinsic deformation behavior of HEAs.

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Heterostructured Fe-Based alloys with unprecedented soft-magnetic properties and manufacturability

Fe-based alloys with a nanocrystalline-amorphous heterostructure exhibit superior soft-magnetic performances; however they generally suffer from the low magnetization because of their heavy doping for an acceptable manufacturability. Here, we report a revolutionary heterostructure-construction concept based on preforming dense nuclei in the melt-quenching process with a critical cooling rate and refining the nano-structure via transient metalloid-rich interfaces. Novel FeBSiPC alloys were developed via our high-entropy stabilization and critical formability strategies by using a total of only 4.6 wt. % light metalloids. This unique alloy design effort leads to unprecedented magnetic properties with the super-high Bs of 1.87 T and μe of 1.0-2.5×104, which outperform all commercial counterparts and have a high potential to substitute for commercial bulk Si-steels currently used for soft-magnetic applications. The unique hetero-structuring and lean-alloying strategy provide a paradigm for the next-generation of magnetic materials with a synergy of superior properties, high manufacturability and low cost.

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The Cores of the Screw Dislocations in BCC Transition Metals and Alloys

The behaviour of the screw dislocation controls plastic deformation and fracture in BCC transition metals and alloys. With decreasing temperatures, the lattice friction of the screw dislocation increases to gigapascal-levels, making stress-relieving dislocation plasticity difficult and nearly all BCC transition metals brittle. This temperature-dependent behaviour is governed by the core of the h111i/2 screw dislocation, the nature and control of which have been studied for decades. We recently discovered that the screw core structure and associated properties are controlled by the energy differences between the FCC and BCC structures of the underlying elements. This insight leads to a new material index $\Delta E = E_{FCC} - E_{BCC}$ that captures this critical energy through crystal geometry and atomic bonding. For BCC transition metal alloys, this index can be normalized as $\chi = \Delta E^A/\Delta E^P$, where superscripts A/P represent alloyed/pure BCC transition metals. The lattice friction and nucleation barrier have near-linear scaling with χ and the core transforms from non-degenerate to degenerate when χ drops below a threshold in BCC alloys. χ is universally applicable to all BCC (alkali and transition) elements across the entire periodic table and all BCC alloys. We demonstrate the validity of χ through (i) extensive DFT calculations of core structures and properties in conventional binary BCC transition metal alloys and emerging multi-principle element complex alloys; (ii) core structure calculations by all empirical/semi-empirical interatomic potentials developed up to date and (iii) comparisons of predicted hardening/softening and slip behaviour with a broad range of extant experiments. χ can be quantitatively and efficiently predicted via rapid DFT calculations for any BCC alloy/composition, providing a robust, easily applied tool for the design of ductile and tough BCC alloys.

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Heterogenous columnar-grained high-entropy alloys produce exceptional resistance to intermediate-temperature intergranular embrittlement

High-entropy alloys (HEAs) strengthened by coherent nanoparticles show great potentials for elevated-temperature structural applications, which however, generally suffer from a severe intergranular embrittlement when tested at intermediate temperatures (around 600-800 °C). In this study, we demonstrated a novel "heterogenous columnar-grained" (HCG) approach that can effectively overcome this thorny problem. Different from the equiaxed counterpart which shows extreme brittleness along grain boundaries at 800 °C, the newly developed HCG-HEA exhibits an exceptionally high resistance to intergranular fractures originating from the unique grain-boundary characters and distributions. The presence of heterogenous columnar grain structure drastically suppresses the crack nucleation and propagation along with boundaries, resulting in an unusually large tensile ductility of ~18.4 % combined with a high yield strength of ~652 MPa at 800 °C. This finding provides a new insight into the innovative design of high-temperature materials with extraordinary mechanical properties.

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Novel heterogeneous lattice strain strengthening in severely distorted crystalline solids

Multiprincipal element alloys (MPEAs) exhibit outstanding mechanical properties owing to the core effect of severe atomic-lattice distortion distinctly different from traditional alloys. However, at the mesoscopic scale, the underlying physics for the abundant dislocation activities responsible for strength-ductility synergy has so far not been uncovered. While the Eshelby mean-field approaches become insufficient to tackle yielding and plasticity in severely distorted crystalline solids, here we develop a novel three-dimensional discrete-dislocation dynamics simulation approach by taking into account the experimentally measured lattice-strain field from a model FeCoCrNiMn MPEA to explore the heterogeneous-strain-induced strengthening mechanisms. Our results reveal that the heterogeneous lattice strain causes unusual dislocation behaviors (i.e., multiple kinks/jogs, and bidirectional cross slips), resulting in the strengthening mechanisms that underpins the strength-ductility synergy. The outcome of our research sheds important insights into the design of strong-yet-ductile distorted crystalline solids, such as high-entropy alloys and high-entropy ceramics.

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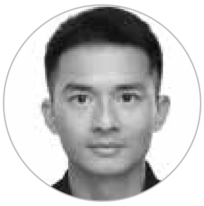
Multiscale discrete dislocation dynamics study of gradient nano-grained materials

Gradient nano-grained (GNG) metals have shown a better strength-ductility combination compared to their homogeneous counterparts. In this paper, the mechanical properties and the related deformation mechanisms of GNG aluminum were investigated using three-dimensional multiscale discrete dislocation dynamics (DDD). GNG polycrystalline models and uniform nano-grained (UNG) counterparts were constructed within a multiscale DDD framework. A dislocation-penetrable grain boundary model based on a coarse-graining approach was adopted to handle the interaction between dislocations and grain boundaries. The simulation results show that the yield stress and strain hardening of the GNG sample is larger than the value calculated by the rule of mixtures, indicating a synergetic strengthening induced by the gradient structure. The associated microstructure evolution demonstrates that dislocations initially activate and glide in the larger grains and then gradually propagate into the smaller grains in the GNG sample, this sequential yielding of layers with different grain sizes generates stress and strain gradients, which is accommodated by geometrically necessary dislocations (GNDs). Moreover, we found that the Bauschinger effect in GNG sample is stronger than those in component UNG samples, suggesting a significant back stress strengthening in the GNG sample during plastic deformation. Finally, a theoretical model is established which successfully describes the Bauschinger effect of GNG and corresponding UNG samples according to the features of dislocation evolution upon unloading. The present study provides insights into the outstanding mechanical property of GNG metals from the view of dislocation dynamics at the submicron scale and offers theoretical guidance for designing strong-and-ductile metals.



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Multiscale modeling of heterostructured materials

Multiscale modelings have been performed to reveal the deformation mechanisms and quantitatively correlate the microstructure with the macroscopic mechanical response of heterostructured materials. A continuum model of dislocation transport incorporating GB transmission was developed in a dislocation-based crystal plasticity framework, which was then adopted to study the deformation mechanisms of gradient-structured material. The nonlocal nature of the model on the slip system level enables the direct investigation of strain gradient effects caused by internal deformation heterogeneities. Furthermore, the interaction between dislocations and grain boundaries leads to the formation of pileups near grain boundaries, which is key to studying the grain size effects in polycrystals. Finite element implementation of the model for polycrystals with different grain sizes captured the grain size effect well. Simulation results of gradient-structured materials and their homogeneous counterparts showed that smaller grains lead to higher geometrically necessary dislocation density and enhanced back stress. Based on the revealed mechanisms, a dislocation density-based strain gradient constitutive model was developed, in which the evolution laws for the widely-concerned geometrically necessary dislocation density and back stress were constructed by means of the dislocation pileup configuration. Finite element implementation of this model quantitatively captured the tensile responses of gradient-structured material and laminated materials with various microstructures. This work helps to understand the contributions of deformation mechanisms to the synergetic strength and ductility of heterostructured materials and to guide the microstructure design and optimization for improved strength-ductility combination.

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Manipulating three- and zero-dimensional defects in heterostructured gradient materials

For heterostructured gradient materials, the engineered heterogeneity or gradient is mainly about two- and one-dimensional crystal defects such as intergranular and interphase boundaries, and dislocations, respectively. In this talk, we will present our recent studies of employing high-pressure torsion (HPT) technique in manipulating three- and zero-dimensional defects, namely, gas-filled pores in metals and oxygen vacancies in oxides, respectively. Sub-nanosized (1-10 nm) nitrogen-filled pores were introduced to copper during HPT process, and contributed to extraordinarily high thermostability in the ultrafine-grained Cu sample. In the other study, we uncover a gradient of oxygen vacancy concentration and concomitant bandgap narrowing in an individual zinc oxide nanoparticle processed by HPT.

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Microstructure and mechanical properties in Ti-Nb-Zr alloy-based composites, reinforced by boride particles

Titanium alloys of the Ti-Nb-Zr system have a low modulus of elasticity, high specific strength, excellent corrosion resistance and biocompatibility, which determines their widespread use in implantology, traumatology and orthopedics. However, the use of these alloys is often limited by relatively low strength, hardness and wear resistance. A significant improvement in strength characteristics can be achieved by creating metal-matrix composites with ceramic reinforcing components. The best choice for titanium-based alloys is hard TiB particles which match well to the titanium matrix without the formation of a transition region; in addition, due to its good thermal stability and similar coefficient of thermal expansion, TiB can operate as an effective reinforcement at elevated temperatures. Meanwhile one of the possible modification of the matrix can be associated with the transition to a medium-entropy composition due to which additional strengthening mechanisms can be expected.

The TiNbZr alloy-based composites with different amounts of borides (1.0, 6.8 and 13.2 vol.%) were produced by vacuum arc melting. The microstructure of the composites comprised the bcc TiNbZr matrix and needle-like (Ti, Nb)B particles with the average thickness of 0.2, 1.1 and 2.4 μm, respectively. Besides ω phase particles measured ~ 10 nm were found in the matrix. The minimum content of borides did not have noticeable effect on the mechanical properties of the composite in comparison with the equatomic TiNbZr alloy. An increase in the amount of borides to 6.8% vol.% resulted in an increase in the yield stress by 22% without a decrease in plasticity. Additional 30% increment in strength (to YS=1010 MPa) with a considerable decrease in ductility (9% height reduction before fracture) was observed for the composite with 13.2% of (Ti, Nb)B. Contributions of different mechanisms into the overall strength were evaluated.

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Transient confinement of the quaternary tetramethylammonium tetrafluoroborate salt in nylon 6,6 fibres: structural developments for high-performance properties via a temporal weakening of the hydrogen bonds

A temporal confinement of the quaternary tetramethylammonium tetrafluoroborate (TMA BF_4) salt among the polyamide molecules has been used for the preparation of high-modulus and highstrength properties of aliphatic polyamide nylon 6,6 fibres. In this method, the suppression or the weakening of the hydrogen bonds between the nylon 6,6 segments has been applied during the conventional low-speed melt spinning process. Thereafter, after the complete hot-drawing stage, the quaternary ammonium salt is fully extracted from the drawn 3% wt salt-confined fibres (by using pentahydrate sodium thiosulphate, $Na_2S_2O_3.5H_2O$, solution) and the nascent fibres are, subsequently, thermally stabilized (under tension). The structural developments that are acquired in the confined-nylon 6,6 fibres are ascribed to the developments (improvements) of the overall fibres' properties due to the confinement process. Surprisingly, unlike the neat nylon 6,6 fibres, the XRD patterns of the as-spun salt-confined fibres have shown diminishing of the (110)/(010) diffraction plane that obtained pseudohexagonal-like β' structural phase. Moreover, the β' pseudohexagonal-like to α triclinic phase transitions took-place due to the hot-drawing stage (draw-induced phase transitions). Interestingly, the hot-drawing of the as-spun salt-confined nylon 6,6 fibres achieved the same maximum draw ratio of 5.5 at all of the drawing temperatures of 120, 140 and 160 ^{o}C. The developments that happened produced improved values of 43.32 cN/dtex for the tensile modulus and 6.99 cN/dtex for the tensile strength of the reverted fibres. The influences of the TMA BF_4 salt on the structural developments of the crystal orientations, on the morphological structures and on the improvements of the tensile properties of the nylon 6,6 fibres have been systematically studied.

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Fabrication of heterogenous layered structure with selective laser melting additive manufacturing

Hetero-structuring is considered as one of the effective strengthening routes in metallic materials to realize excellent strength-ductility synergy. This strengthening effect can be achieved by heterogeneous regions which have different mechanical property or microstructural characteristics. Among various type of additive manufacturing process, selective laser melting (SLM) is a key technology which can fabricated parts with complex shape that can't be achieved with conventional process. Furthermore, various process conditions of SLM can be used to control the mechanical properties and micro structure.

In this work, we demonstrate a new capability of selective laser melting in controlling the site-specific microstructures and developing architectured heterogeneous materials. With popular 316L stainless steel, heterostructured layered sample was fabricated where multiple process parameter was applied to multiple region. Fabricated layered structure demonstrated an excellent combination of strength and ductility compared to homogeneous materials. The current approach is versatile and can be used for many printable alloys. Further, this work can be expanded 3 dimensionally so this approach opens a new direction in metal additive manufacturing to produce heterostructured materials for enhanced strength and ductility.

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Effect of Al_2O_3 doping on microstructure evolution and densification process of AZO targets

The main objective of this work is to investigate the effect of aluminum doping on the sintering activity of zinc oxide ceramic targets. The pressure slip casting was used to prepare the green ZnO and AZO compacts with high density and uniformity. The densification and grain growth activation energy of pure ZnO and AZO ceramic targets were calculated, and the effects of traditional sintering and two-step sintering on the grain size and density of the ceramic targets were studied in detail. The results demonstrated that the ceramic AZO target with a relative density of 99.8% and a grain size of 3.89 μm was obtained by the two-step sintering method.

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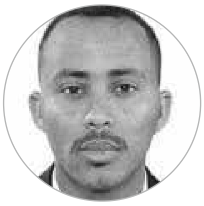
Ultra-high tensile strength via precipitates and enhanced martensite transformation in a FeNiAlC alloy

The aging and quenching at critical temperatures of a hot-rolled (HR) Fe-Ni alloy was studied to obtain B2 precipitates with a variety of volume fractions and sizes. The yield strength and strain hardening of the aged samples were higher than those of the HR sample, and the corresponding deformation mechanisms were studied in detail. The aged samples exhibit stronger hetero-deformation-induced hardening than the HR samples. The phase transformation during tensile testing is much easier on aged samples than on HR samples. This can be attributed to the high local stress caused by the B2 precipitates surrounding the austenite grains and the reduced stability of austenite due to nickel and aluminum diffusion during aging. The deformation-induced lath martensite can be observed after tensile deformation, with the high-density dislocations rendering a significant strain hardening. Moreover, the density of twins increases visibly in the martensite after tensile deformation, contributing to the strain hardening following the dynamic Hall-Petch effect.



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Effects of electron beam irradiation crosslinking on microstructure and electrochemical performance of hybrid polyethylene separators for lithium-ion batteries

The new generation of rechargeable batteries, such as lithium-ion batteries (LIB), should not only have faster rate capability and higher energy density than present batteries but also should be environmentally friendly, safe, and low-cost. In recent years, the research of LIBs has attracted worldwide attention because of its broad application prospects in various next-generation energy storage devices such as mobile phones, camcorders, notebook computers, power tools, hybrid vehicles, and robots. The separator is an important component of LIBs because it avoids physical contact between electrodes (cathode and anode) while allowing the passage of ions between them. To date, several attempts have been done to modify microporous separators, However, modification of separators to increase safety, improve electrochemical performance, and commercially lower their cost remains challenging. Herein, we aimed to manufacture commercial nanocomposite membranes between ultra-high molecular weight polyethylene (UHMWPE) and silicon dioxide (SiO_2) via the biaxial stretching technique, subsequently applying the high-energy E.B irradiation for crosslinking without post-treatments toward overcoming the limitations of commercial separators and improving the electrochemical performance. In addition, the impacts of the E. B irradiation crosslinking on the mechanical properties, thermal stability, as well as electrochemical performances of both UHMWPE (M1) and UHMWPE-SiO_2 (M2) separators were intensely studied. Furthermore, the requirements of separators, including tensile strength, Young's modulus, thermal stability, air permeability, electrolyte uptake, porosity, ionic conductivity, and rate capabilities, were systematically studied and compared. According to our findings, E.B irradiation crosslinking improved the properties of both nanofibrous M1 and nanocomposite M2 separators, so that these two modified separators have outstanding electrolyte uptake capacities and excellent ionic conductivities. As a result, E.B crosslinked M1 and M2 separators withstood higher current densities and longer cycle periods than the non-cross-linked versions. Therefore, this work offers a viable and cost-effective method for producing and modifying commercial separators to improve LIBs' safety and stability.

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Effect of hardening with borides on the microstructure and mechanical properties of Al5Nb24Ti40V5Zr26 alloy-based composites

The issue of increasing the strength characteristics, hardness and wear resistance of beta titanium alloys while maintaining or reducing the elastic modulus is relevant, since this would significantly expand the scope of these materials. A radical improvement in the strength characteristics of titanium alloys can be achieved by using a combination of different hardening strategies, both through a significant modification of the chemical composition and the transition to the high-entropy compositions, and through the creation of metal-matrix composites with ceramic reinforcing components, for example, particles of titanium borides.

In this work the Al5Nb24Ti40V5Zr26 alloy-based composites with different amounts of reinforcing component TiB_2 were produced by vacuum arc melting in a high purity argon atmosphere. For melting, pure (with a purity of at least 99.9%) elements that make up the matrix, as well as TiB_2 powder with an average particle size of 3-8 microns, were used. The weight proportion of TiB_2 in cast composite billets was 1, 2 and 3 mass. %. In the as-cast condition composites had a single phase bcc structure. The microstructure of the alloy in the initial condition consisted of mainly equiaxed grains with a size of ~ 100 µm with needle-like monoborides (Ti, Nb) B heterogeneously distributed within the bcc matrix. After tensile testing at room temperature, the sample reinforced 1 mass. % TiB_2 showed a yield strength of 840 and an elongation of 5. It is worth noting that that increasing the content of the reinforcing component TiB_2 to 2 and 3 mass. % leads to a sharp drop in ductility (0.5 and 0 %, respectively) and a slight increase in strength: the value of the yield strength was 890 and 900 MPa, respectively.

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Mechanical propertied and deformation behavior of novel refractory high-entropy alloys with a BCC-B2 structure

Conventional paradigm says that intermetallic should be embedded as coherent reinforcements in a disordered and soft matrix to ensure balanced mechanical properties. When intermetallics stand as a matrix, alloys are anticipated to be strong yet brittle. For instance, in the recently developed refractory high-entropy alloys (RHEAs), a mixture of an intermetallic B2 matrix and coherent bcc particles provided high strength at elevated temperatures but low room-temperature plasticity. Meantime, several works reported that some B2 phases, namely Co-X (X = Ti, Zr, Hf), could be ductile even under tension at room temperature. These compounds had high melting points, albeit they showed low yield strength. In this study, we demonstrated that body-centred cubic particles could strengthen such B2 compounds in a quite unexpected manner. The resulted heterogeneous, dual-phase structure ensured a better strength-plasticity combination compared to initial single-phase counterparts. The composition-structure-property relationships and possibilities for further improvements of properties are discussed.

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Formation of a heterogeneous microstructure in a medium entropy alloy of the Fe-Co-Ni-Cr-C system

It is well known that high entropy alloys (HEAs and MEAs) have an almost infinite compositional area to create materials that allow opening more diverse microstructures with improved mechanical properties. This work presents studies of the microstructure and mechanical properties of one of the medium entropy alloys of the Fe-Co-Ni-Cr-C system, obtained by a modern method of additive technologies.

The $Fe_{65}(CoNi)_{25}Cr_{9.5}C_{0.5}$ alloy was obtained by selective laser sintering (melting). The microstructure of the alloy was studied using transmission and scanning electron microscopy and EBSD analysis. Tensile tests were carried out to evaluate mechanical properties.

The alloy in the initial as-printed state has a two-phase structure (fcc - 99% and a small fraction of bcc - 1%). During tensile tests at cryogenic temperatures, the alloy exhibits the so-called TRIP effect (transformation-induced plasticity). The tensile strength of the alloy reaches a high value (σB = 1801 MPa), while its relative elongation to failure remains at a decent level (δ = 27%). Examination of the alloy after tensile tests showed the formation of a heterogeneous microstructure due to the fcc-to-bcc martensite transformation. The amount of the fcc phase decreased to 9%, while the percentage of the bcc martensitic phase increases to 91%. The development of the TRIP effect in the as-printed $Fe_{65}(CoNi)_{25}Cr_{9.5}C_{0.5}$ alloy is discussed in more detail.

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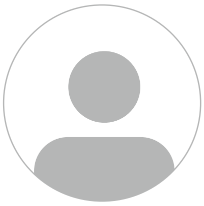
Cold sintering of ceramic materials

The demand of ceramic composites for multifunctional devices is rapidly increasing. Sintering ceramics usually needs a temperature of over 1000°C. To reduce the quantity of heat generated, a novel sintering method named cold sintering process, based on the use of a temporary solvent and the use of pressure has been devised. It may sinter oxides, carbonates, bromides, fluorides, chlorides, and phosphates. The performances of electronic materials can be tailored by forming heterogeneous composites through cold sintering process. The mechanisms of microstructural development, cold sintering of ceramic composites and the physical properties are discussed in this study.



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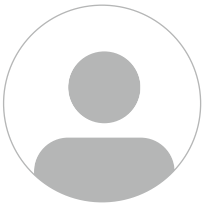
The effect of nitrogen on the structure and mechanical properties of the $Fe_{40}Mn_{40}Cr_{10}$-Co_{10}-based alloys

High-entropy alloys (HEAs) with a face-centered cubic (FCC) structure are currently considered as promising structural materials. The Co-Cr-Fe-Mn-Ni system alloys demonstrated encouraging properties, for example, high ductility and fracture toughness at room and cryogenic temperatures, but generally they have low strength. The $Fe_{40}Mn_{40}Cr_{10}Co_{10}$ alloy is particularly interesting as a single-phase solid solution with impressive mechanical properties. Thermomechanical processing can be effectively used to tailor the microstructure and properties. In addition, alloying with interstitial elements, in particular nitrogen, can lead to significant hardening. Therefore, in this work the effect of nitrogen content (0; 1 at.%) on the structure and mechanical properties of the $Fe_{40}Mn_{40}Cr_{10}Co_{10}$-based alloys after thermomechanical processing was studied.

The $Fe_{40}Mn_{40}Cr_{10}Co_{10}$ alloy had dual-phase structure with FCC matrix and sigma phase precipitates, while N-doped alloy had single-phase FCC structure. Nitrogen alloying increases both strength and ductility at room temperature. Decrease in the testing temperature results in the pronounced increase in strength of the alloys. Heterogeneous structure formed in the $Fe_{40}Mn_{40}Cr_{10}Co_{10}$ after cold rolling with subsequent annealing. Sigma phase fraction decreased with the increase in the annealing temperature. Some M_2N type nitrides were found in $Fe_{39}Mn_{40}Cr_{10}Co_{10}N1$ alloy after annealing at 700°C. After annealing at higher temperatures, the alloy had a single-phase FCC structure. The microstructure-mechanical properties relationships and effect of nitrogen strengthening mechanisms is discussed.



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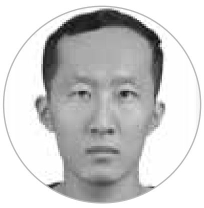
Microstructure and mechanical behavior of al-doped CoCrFeMnNi with dual-phase FCC/B2 structure

High entropy alloys (HEAs) based on the well-known Cantor CoCrFeMnNi alloy are known for their exceptional ductility and damage tolerance, especially in cryogenic conditions. However, the strength of these alloys with a single face-centered cubic (fcc) phase is often insufficient for practical application. More balanced properties can be obtained when additional hard phases are added. For example, alloying with Al can result in the precipitation of a hard B2 phase particles in the soft fcc matrix. However, proper tailoring of the microstructure and mechanical properties require careful control over chemical composition and processing condition.

In the present work, the CoCrFeMnNi-type doped with ~8 at.% of Al was studied. In the as-cast condition the alloy had almost entirely single fcc phase structure with insignificant amount of the B2 particles. The-as-cast alloy had low strength but high ductility. The alloy was cold rolled and annealed at 800 and 900˚C for different duration (1 min - 50 hours). As a result, fully or partially recrystallized fine-grained fcc matrix with a significant amount (~20%) of the B2 particles was produced. Such a complex microstructure promoted high strength (ultimate tensile strength up to 1300 MPa) with reasonable ductility. The microstructure evolution is analyzed in details with a fucus on interplay between the precipitation of the B2 phase particles and recrystallization in the fcc phase. Microstructure-mechanical properties relationships are also discussed.



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{112}<111> Twins or twinned variants induced by martensitic transformation?

Martensitic transformation has been deeply investigated for centuries, however, some issues remain controversial. Among them, twinned substructure is of particular interest, since it represents a category of martensite with broad applications. However, the origin of twinned substructures in martensite and the existence of secondary phases at twin boundaries are still highly debated. In the present investigation, twinned substructure in lath martensite was induced in IF steel via a high pressure thermal cycle (heating up to 1100 ˚C and holding for 30 min, cooling at 10 ˚C/s to room temperature under a pressure of 4 GPa). Experimental observations and theoretical simulation confirm that the twinned substructure has the origin related to the twinned variants rather than the bcc {112} twins, while extra diffraction spots were caused by crystal overlapping rather than any extra phase. The differences in crystallography and electron diffraction behavior between twinned variants and {112} twins were discussed in detail.

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