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GENERAL INFORMATION

Venue

Rm. S104, Teaching Building, UCAS, Zhong-Guan-Cun Campus
Add: No.3 Nanyitiao, Zhongguancun, Haidian District, Beijing, P.R.China
Website: http://2017slg.csp.escience.cn

A map of KITS and its neighborhood including location of hotels can be found at the back of this handbook

Registration

The registration desk will be opened at the UCAS, Zhong-Guan-Cun Campus during the following hours:
1500-1800, 6 August 2017
0830-1700, 7-18 August 2017

Presentation Preparation

Presenters must upload presentations during coffee breaks before, preferably one day prior to the start of their session to ensure their presentations are loaded successfully

Internet-Wireless

All delegates have access to the UCAS free wireless Internet service. The user name and password will be announced during the conference

Catering

Morning and Afternoon Tea Breaks
Tea breaks during the conference will be served outside Rm. S104, Teaching Building

Welcome Banquet
1830, (Buses departure at 1800 from the UCAS, Zhong-Guan-Cun Campus), Quanjude Restaurant, 6 July.
(invitation card required)

Nearby Cafes and Restaurants
IOP Café can be found at 9th floor, IOP M Building next to KITS. There are also numerous cafes and restaurants near KITS. Have fun with Chinese food and language!

CONFERENCE PROGRAM

Week 1

August 7, 2017, Monday

08:30-09:00 **Fu-Chun Zhang,** KITS, UCAS
Opening Session, Introduction to KITS

Morning Session Chair: K. L. Ngai
09:00-09:45 **Haibin Yu,** Huazhong University of Science and Technology
Molecular dynamics simulations of dynamical mechanical spectroscopy in metallic glasses: linear and nonlinear responses

09:45-10:10: ***Coffee Break***

10:10-10:55 **Jepp Dyre,** Roskilde University
Identifying the material time in physical aging

10:55-11:40 **Tianhui Zhang**, Soochow University
Continuous Structural evolution of nucleation in colloids

August 8, 2017, Tuesday

Morning Session Chair: Yujie Wang
09:00-10:00 **Walter Kob,** University of Montpellier
Probing the properties of ideal glasses

10:00-10:20 ***Coffee Break***

10:20-11:05 **Zhaoping Lv,** University of Science and Technology Beijing
Unique glass-glass transition in Pd-based metallic glasses

11:05-11:50 **Yue Wu**, University of North Carolina
Non-Density Driven Liquid-Liquid Transition

August 9, 2017, Wednesday

Morning Session Chair: Walter Kob

09:00-09:45 **Mingwei Chen,** Johns Hopkins University
TBD

09:45-10:10 ***Coffee Break***

10:10-10:55 **Cai-Zhuang Wang**, Ames National Lab
Local structure orders in metallic liquids and glasses and their influences on the dynamics of glass and phase selections

10:55-11:40 **Kang Chen,** Soochow University
Nonlinear Langevin Equation Theory and its application to colloidal polymer glass

18:00-20:00 **Dinner Banquet at Peking Duck Restaurant**

August 10, 2017, Thursday

Morning Session Chair: Cai-Zhuang Wang

09:00-10:00 **Lanhong Dai,** Institute of Mechanics, Chinese Academy of Sciences
Towards dilation in flow and fracture of metallic glasses

10:00-10:20 ***Coffee Break***

10:20-11:05 **Gang Wang,** Shanghai University
Discontinuous Deformation Behavior in Metallic Glasses

10:05-11:50 **Jie Zhang**, Shanghai Jiao Tong University
Study of an athermal quasi-static plastic deformation in a 2D granular material

August 11, 2017, Friday

Morning Session Chair: Yue Wu

09:00-09:45 **Yujie Wang,** Shanghai Jiao Tong University
Granular packing as model glass formers

09:45-10:10 ***Coffee Break***

10:10-10:55 **Pengfei Guan**, Beijing Computational Science Research Center
A Link between Structural Relaxation and Dynamic Heterogeneity in Glass-Forming Liquids

10:55-11:40 **Maozhi Li**, Renmin University of China
five-fold local symmetry in metallic liquids and glasses

Week 2

August 14, 2017, Monday

Morning Session Chair: Jeppe Dyre

09:00-09:45 **K. L. Ngai,** University of Pisa
TBD

09:45-10:10 ***Coffee Break***

10:10-10:55 **Rafi Blumenfeld**, NUDT and Imperial College
Entropy in disordered particulate systems

10:55-11:40 **Ke Chen**, Institute of Physics, Chinese Academy of Sciences
Defects and structural order in colloidal glasses

August 15, 2017, Tuesday

Morning Session Chair: Ke Chen

09:00-09:45 **Yilong Han**, Hong Kong University of Science and Technology
Making glasses from crystals or vapors

09:45-10:10 ***Coffee Break***

10:10-10:55 **Zhongyu Zheng,** Institute of Mechanics, Chinese Academy of Sciences

Glass transition in monolayers of colloidal ellipsoids

10:55-11:40 **Zexin Zhang,** Soochow University
Glassy Dynamics in Two-dimensional Melting

August 16, 2017, Wednesday

First Morning Session Chair: Rafi Blumenfeld

09:00-09:45 **Peter Harrowell,** University of Sydney
Dynamic Heterogeneities and the Distribution of Constraint in Supercooled Liquids

09:45-10:30 **Bo Zhang**, Hefei University of Technology
Inter-diffusion and self-diffusion in liquid $Ce_{80}Ni_{20}$

10:30-10:45 ***Coffee Break***

Second Morning Session Chair: Corey O'Hern

10:45-11:30 **Xiaohua Zhang,** Soochow Univeristy
Glass Transition of Polymer in Nanochannels

11:30-12:15 **Peng Tan,** Fudan University
Complex Structures and Dynamics Resulted from Long-range Anisotropic

August 17, 2017, Thursday

Morning Session Chair: Xunli Wang

09:00-09:45 **Yanhui Liu**, Institute of Physics, Chinese Academy of Sciences
Discover better metals faster-A case study on metallic glasses

09:45-10:10 ***Coffee Break***

10:10-10:55 **Zhefang Zhang**, Institute of Metal Research, Chinese Academy of Sciences
Fracture mechanisms and strength theory of metallic glasses

10:55-11:40 **Corey O'Hern**, Yale University
Mechanical properties of glasses: Rearrangement statistics and measures of Ductility

August 18, 2017, Friday

Morning Session Chair: Jie Zhang

09:00-09:45 **Xunli Wang**, City University of Hong Kong
Cluster connectivity and medium range order

09:45-10:10 ***Coffee Break***

10:10-10:55 **Nicolas Giovambattiste**, City University of New York
Understanding Water Polymorphism using the Potential Energy Landscape Approach

10:55-11:40 **Zhenwei Wu**, Peking University
Local connectivity modulates multi-scale relaxation dynamics in a metallic glass-forming system

11:40-12:00 **Wei-hua Wang,** Institute of Physics, Chinese Academy of Sciences
Closing remarks

ABSTRACT CONTENTS

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Molecular dynamics simulations of dynamical mechanical spectroscopy in metallic glasses: linear and nonlinear responses

HaiBin Yu (HUST)

Relaxation dynamics are the central topics in glassy physics. They are usually measured by the experimental techniques of dynamical spectroscopies such as the dielectric and mechanical spectra. Here, we put the protocols of the dynamical mechanical spectroscopy into molecular dynamics simulations. It reproduces the salient features of relaxation spectra as measured experimentally. Moreover, combining it with detailed studies atomic movements and structural analysis, we clarified the mechanisms of internal friction of metallic glasses [1]. We observed the strain driven glass transition and a pronounced fragility transition as induced by nonlinear strain [2]. We find that the primary (α) relaxation always takes place when the most probable atomic displacement reaches a critical fraction (~20%) of the average interatomic distance, irrespective of whether the relaxation is induced by temperature (linear response) or by mechanical strain (nonlinear response) [3].

Reference

[1] H.-B Yu and K. Samwer, Phys. Rev. B **90**, 144201 (2014).

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Identifying the material time in physical aging

Jeppe C. Dyre (Roskilde Univ.)

In 1971 Narayanaswamy - an engineer at Ford Motor Company - proposed the simple, yet powerful theory of physical aging that is today used routinely industry all over the world [1]. Aging of glasses is known to be a highly nonlinear process, but according to what soon became known as the Tool-Narayanaswamy (TN) theory, aging is described by a linear time-convolution integral if time is replaced by the so-called material time. The TN theory is highly successful, e.g., for describing relaxation following small or moderate sized temperature jump, and the theory has been applied routinely in industry for decades. Nevertheless, there have been only few attempts to justify the TN formalism from first principles. The talk briefly reviews the TN formalism and shows recent data confirming the theory in a novel, simplified form [2]. Interestingly, this form leads to a differential equation for the relaxing quantity as a function of time, even though the great leap forward provided by Narayanaswamy was to move away from differential equations. We briefly resolve this enigma. Finally, we show that the material time is determined by the distance squared to a configuration of the system's distant past [3].

Reference

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2. T. Hecksher, N. B. Olsen, and J. C. Dyre, J. Chem. Phys. 142, 241103 (2015).
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Continuous Structural evolution of nucleation in colloids

Tian Hui Zhang (Soochow Univ.)
Jing Sheng Cao (Soochow Univ.)
Xiang Yang Liu (FOS, NUS)

Nucleation will not only determine if the phase transition will happen, but also the structure of the new phase that occurs. The rate of nucleation is associated with the free energy barrier-so-called nucleation barrier, which is determined by various factors, including the structure of the nucleating phase. Within the framework of classical nucleation theory, the structure of nuclei is identical to that of bulk crystals, and regarded as a constant parameter in the kinetics. However, it follows from the recent studies that, nuclei are often observed in multi-step processes: they initially form as a metastable structure, and transformed into a more stable one subsequently. Nevertheless, the multi-step structure evolution of nuclei and the impact on nucleation kinetics have never been examined. In this study, we report a detailed study on the kinetics of nucleation with a continuous structure evolution based on in-situ observation on controlled colloidal crystallization. It follows that the structure of nuclei experiences a continuous transition from disordered to ordered. Initially, pre-critical nuclei form with a liquid-like structure. In the following growth, the liquid-like nuclei begin to nucleate crystalline structure inside via fluctuation and a stable crystalline core is created successfully till the nuclei cross over a critical size. In this process, the crystallinity of nuclei in terms of the fraction of crystal-like particles increases continuously. A quantitative model based on particle bonding shows that the continuous structure transition of nuclei gives rise to a much lower nucleation barrier than that in a one-step abrupt transition. Upon the increase of supersaturation, the disordered-ordered transition occurs abruptly at the birth of nuclei as the nucleation barrier vanish. It demonstrates that the pathway of nucleation is supersaturation-dependent: multi-step nucleation or continuous evolution of nuclei in principle is favored as a high nucleation barrier has to be overcome.

Probing the properties of ideal glasses

Walter Kob (Univ. of Montpellier)

More than 60 years ago Kauzmann found evidence that glass-forming systems might have a thermodynamic singularity at a temperature that today is referred to as the "Kauzmann temperature". Soon after this discovery it became obvious that probing the properties of such a putative ideal glass-transition might be difficult, or even impossible, since this critical temperature lies below the experimental glass transition temperature, thus forbidding to study the equilibrium properties of the liquid in the temperature range of interest. Only very recently new theoretical ideas have been put forward that might allow to probe the equilibrium properties of a glass-forming system in the vicinity of its Kauzmann temperature. In my talk I will discuss this idea and present the results of computer simulations that do indeed give evidence that certain glass-formers show at sufficiently low temperatures a thermodynamic transition. Finally I will discuss the relaxation dynamics of the glass-former in the vicinity of this transition and show that even in the ideal glass state this dynamics is not completely frozen.

Unique glass-glass transition in Pd-based metallic glasses

Q. Du, X. J. Liu, **Z. P. Lu** (USTB)

Analogous to the well-known polymorphism in crystalline materials, polyamorphic transition (PT) is also observed often in amorphous matters. For metallic amorphous alloys, however, PT remains rare and poorly understood. Herein we report the discovery of two abnormal polyamorphic transition behaviors in Pd-based metallic glasses:

1) Thermal driven glass-glass transition behavior upon heating

   An unique glass-glass transition under ambient pressure was observed upon heating Pd-based MGs to above their glass transition temperature. Our results demonstrate a first-order PT into a new and deeper energy megabasin, characterized by an exothermic peak in calorimetric scan, together with a precipitous drop in volume, electrical resistance and specific heat, as well as clear evidence of local structural ordering on the short-to-medium-range scale revealed via in-situ synchrotron X-ray scattering. Atomistic simulations indicate enhanced ordering of locally favored motifs to establish correlations in medium range that resemble those in equilibrium crystalline compounds.

2) Abnormal glass-glass transition behavior under high pressure

Pressure-induced glass-glass transition has been reported in a few rare-earth-based and Ca-Al MGs, where the changes in electronic structure induced by pressure are believed to be responsible. Phenomenally, the compressibility (i.e., the slope of volume vs. pressure) becomes smaller as the glass transforms from a low-density amorphous (LDA) state to a high-density amorphous (HDA) state. Herein, an unexpected glass-glass transition behavior was discovered in Pd-based MGs under pressure, which is characterized by the increase of compressibility accompanying by the glass-glass transition from the LDA to HAD state. Theoretical investigation reveals that the abnormal pressure-induced glass-glass transition behavior is attributed to the change in bonding types, i.e., some bonds in the Pd-based MGs evolves from covalent-type bonds to metallic bonds under pressure.

Non-Density Driven Liquid-Liquid Transition

Yue WU (Univ. of North California & HUST)

Understanding qualitative changes of thermodynamics in liquids is essential for solving a whole range of challenging problems in condensed matter physics including the nature of structural glass transition. Obvious changes such as density change and decomposition could lead to phase transitions in liquids. However, structural glass transition is a very general phenomenon and no such obvious changes of order parameters (such as density and composition) associated with glass transition have been identified even on the microscopic scale. This often is summed up by the sentiment of frustration: What is changing?

A similar situation exists in a closely related problem, namely, the nature of liquid-liquid transition (LLT). From thermodynamic point of view, a liquid (even a single-element liquid) could undergo a first-order phase transition from one liquid phase to another liquid phase without change of composition, called LLT. Except a few cases such as cerium where the electronic state of the element changes drastically with pressure leading to substantial change in density, LLT remains controversial. It is not obvious if non-density driven LLT could exist and, if it exists, what the associated order parameter could be.

It becomes increasingly clear that structural information carried by pairwise distribution functions is insufficient for describing qualitative changes in liquids including glass transition. It is also inadequate for describing non-density driven LLT. Nuclear magnetic resonance (NMR) is a very sensitive tool for probing structure and dynamics of liquids and it is particularly sensitive to the overall local structures such as clusters, not just to pairwise distributions. Such sensitivity is shown to be very effective in revealing non-density driven LLTs in metallic alloys and other systems. Possible order parameters associated with such non-density driven LLTs will be discussed and it could also have important relevance to the understanding of the nature of glass transition.

Nonlinear Langevin Equation Theory and its application to colloidal polymer glass

Kang Chen (Soochow Univ.)

Nonlinear Langevin Equation theory connects the static structures and correlation functions to the activated dynamics of glass. Here we extend and apply it to study the glassy dynamics of a new type of assembling materials called “colloidal polymers”. These colloidal polymers have advantages over molecular polymers in the visibility and flexibility of tuning, for example, the size and shape of the “monomers”, the interaction, and the bond length. Dense suspension of colloidal polymers will become a very promising ideal model system for exploring the fundamental problems in the glass transition of chain “molecules”. We focus on the effect of bond length. Bond length is generally not considered as a controllable variable for molecular polymers, while it’s tunable for colloidal polymer. We study the static structure and activated dynamics of hard-sphere colloidal polymers. Surprisingly, we find the bond length plays a critical and unique role in many aspects. For instance, the universal relations of the characteristic local lengths and the activated barrier versus the “degree of supercooling”, and the structural relaxation versus local vibrational motion are found to be dependent on bond length and independent of chain length and rigidity. We hope that our findings inspire future experimental and simulation researches on the glassy dynamics of colloidal polymers.

Keywords: glass, colloid, polymer

Towards dilation in flow and fracture of metallic glasses

L. H. Dai (IOM, CAS)

Metallic glasses, due to long-range disorder of atoms, expand locally or globally in response to shear, bearing a resemblance to Reynolds' dilatation of granular media. It has been widely accepted that shear flow is allowed in metallic glasses via a cascade of local dilatation events, which was mainly modeled by Spaepen's free volume theory or Argon's shear transformation theory. The shear-dilatation coupling leads to the pressure (or normal stress) sensitivity of macroscopic failure (flow and fracture) of metallic glasses, which essentially differs from that of their crystalline counterparts. Recently, it has been revealed that the dilatation itself can dominate brittle fracture of metallic glasses, where the crack tip propagates via cavitating events that involve a series of nanovoids nucleation and coalescence with very limited plastic growth. Therefore, the dilatation holds the key to understand the flow and fracture of metallic glasses. In this talk, we attempt to provide a up-to-date review on this aspect, but from a viewpoint of the dilatation. We first review the representative flow modes for metallic glasses, where the shear-dilatation correlation is highlighted. Theoretical as well as atomistic modeling and experimental work on the dilatation degree during shear banding at different stages are all discussed. Typical yielding criteria accounting for the dilatation effect are then described. We further present the atomic-level mechanism for local shear and dilatation events, respectively. Based on the inherent shear-dilatation competition, a united failure criterion is constructed, in which the governing factors to determine the ductile or brittle failure of metallic glasses are revealed.

Keywords: Metallic glass; shear band; fracture

Discontinuous Deformation Behavior in Metallic Glasses

G. Wang (IOM, CAS)

Bulk metallic glasses (BMGs) usually exhibit a discontinued serrated plastic flow behavior after yielding. In this plastic flow, each serration event includes elastic energy accumulation and relaxation, which corresponds to shear bands formation and propagation. The shear band randomly forms on the sample surface and propagates at a very high velocity, which brings out that the distribution of the amplitude of serration events in the plastic flow is inhomogeneous. Since that, the quantitative description of the serrated flow behavior is difficult. Therefore, in the proposed project, we will use the statistic analysis to investigate the plastic dynamics of BMGs. Through changing the loading condition (including strain rate and environmental temperature) and the microstructure (including fully amorphous and the nanocrystal/glass binary phase structures) of BMGs, we will disturb the plastic dynamics and then explore the dynamics evolution process in the spatio and temporal frame. The structural evolution of BMGs will be in-situ observed in a high resolution microscope accompanied with diffraction technique. Digital scattering correlation method will be applied to explore the strain field distribution at the yielding point. Based on shear transformation zone theory, the correlation between plastic strain render medium distribution and plastic dynamics will be elucidated.

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Study of an athermal quasi static plastic deformation in a 2D granular material

Jie Zhang (SJTU)

In crystalline materials, the plasticity has been well understood in terms of dynamics of dislocation, i.e. flow defects in the crystals where the flow defects can be directly visualized under a microscope. In a contrast, the plasticity in amorphous materials, i.e. glass, is still poorly understood due to the disordered nature of the materials. In this talk, I will discuss the recent results we have obtained in our ongoing research of the plasticity of a 2D glass in the athermal quasi static limit where the 2D glass is made of bi-disperse granular disks with very low friction. Starting from a densely packed homogeneous and isotropic initial state, we apply pure shear deformation to the system. For a sufficiently small strain, the response of the system is linear and elastic like; when the strain is large enough, the plasticity of the system gradually develops and eventually the shear bands are fully developed. In this study, we are particularly interested in how to relate the local plastic deformation to the macroscopic response of the system and also in the development of the shear bands. I will discuss the recent progress we have made in understanding the formation of shear bands in amorphous solids.

Granular packing as model glass formers

Yujie Wang (SJTU)

The nature of glass transition has remained a hotly debated issue. Static granular packings are model hard-sphere glass formers. Using x-ray fast CT technology, we systematically investigated the glass transition in granular packings. We focus on the growth of glass order with five-fold symmetry in granular packings and relate the findings to both geometric frustration and random first-order phase transition theories. We also studied the plastic deformation of granular materials under shear and identified the corresponding structural defect and the celmentary plastic event, which can help our understanding of yield transition and shear band formation for amorphous materials in general and also dense granular flows.

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A Link between Structural Relaxation and Dynamic Heterogeneity in Glass-Forming Liquids

Lijin Wang & **Pengfei Guan** (CSRC)
Ning Xu (USTC), W. H. Wang (IOP, CAS)

Despite the use of glasses for thousands of years, the nature of the glass transition is still mysterious1-3. On approaching the glass transition, the growth of dynamic heterogeneity4-6 has long been thought to play a key role in explaining the abrupt slowdown of structural relaxation. However, it still remains elusive whether there is a universal link between structural relaxation and dynamic heterogeneity. Here we unravel the link by introducing a characteristic time scale hiding behind an identical dynamic heterogeneity for various glass-forming liquids. We find the time scale solely corresponds to the kinetic fragility of liquids. Moreover, it leads to universal scaling collapse of both the structural relaxation time and dynamic heterogeneity for all liquids studied, together with a characteristic temperature associated with the same dynamic heterogeneity. The master curve of the structural relaxation time is fitted best with the Vogel-Fulcher-Tammann equation, suggesting the Adam-Gibbs picture7 of the glass transition. Our findings imply that studying the glass transition from the viewpoint of dynamic heterogeneity is more informative than expected.

Entropy in disordered particulate systems

Rafi Blumenfeld (NUDT & ICL)

The formulation of statistical mechanics for particulate systems made jump-started the field as a rigorous branch of soft matter physics. I review briefly the Edwards formalism, which has been extended to cellular and porous materials, point out a problem with the original formulation and how it was overcome. Using the new formulation, I show that there are several types of contribution to the entropy, which clarifies a recent debate in the field. I also present a derivation of an equation of state, relating the volume, the boundary stress and the equivalent of temperatures in these systems.

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Defects and structural order in colloidal glasses

Xiunan Yang, Rui Liu, Mingcheng Yang, Wei-hua Wang, **Ke Chen** (IOP, CAS)

Glasses are also known as disordered solids whose structures exhibit no obvious long range periodicity. On the other hand, it has been proposed that glasses may contain non-periodic amorphously ordered structures that are closely connected to the fundamental dynamical, thermodynamical and mechanical properties of glasses. Searching for signs of such structural orders has been intensively pursued by both theoretical and experimental workers in the field. Using temperature sensitive soft colloidal particles and video microscopy, we measured local structural entropy S2 in quasi-2D colloidal glasses, and its correlations with local dynamics, phonon modes and local deformations. We find that spatial correlation of S2 increases with packing fractions and extends over the range of several particles. Regions with lower local orders are correlated with faster dynamics, softer phonon modes and the propensity to rearrange under external loading, similar to defects, which makes S2 a promising candidate to probe amorphously ordered structures in glasses.

Making glasses from crystals or vapors

Yilong Han (HKUST)

We compressed a 2D binary crystal into a glass. It exhibits a drastic structural change, in contrast to the conventional glass transition from a supercooled liquid where the structure changes little. We identified the boundary between polycrystal and glass from various mechanical, structural, dynamic, and thermodynamic features. In addition, we identified Hall-Petch and inverse-Hall-Petch regimes in 2D polcrystals and three glass regimes. In the second part, we experimentally studied the relaxations of 2D bidispersed colloidal glasses near its surface during and after the vapor deposition. We observed the surface mobile layer at the single-particle level, and further discovered a middle layer which relaxes via large and anisotropic cooperative motions. It released free volumes towards the surface, leaving a more compact bulk glass. This novel relaxation mode in the middle layer cast light on the ultrastable glasses formed by vapor deposition.

Glass transition in monolayers of colloidal ellipsoids

Zhongyu Zheng (IOM, CAS)

When a liquid is supercooled towards the glass transition, its dynamics drastically slows down, whereas its static structure remains relatively unchanged. Finding a structural signature of the dynamic slowing down is a major challenge, yet it is often too subtle to be uncovered. Here we discover the structural signatures for both translational and rotational dynamics in monolayers of colloidal ellipsoids by video microscopy experiments and computer simulations. The correlation lengths and fluctuations of the dynamic slowest-moving clusters, the dynamic heterogeneity, the static glassy clusters, and the local structural entropy all follow the same power-law divergences towards the ideal glass transition point. It suggests that the kinetic slowing down is caused by a decrease in the structural entropy and an increase in the size of the glassy cluster. Ellipsoids with different aspect ratios exhibit single-step or double-step glass transitions with distinct dynamic heterogeneities. These findings demonstrate that the particle shape anisotropy has important effects on the structure and dynamics of the glass. The different glassy structures underlying the dynamic slowness and heterogeneity at different aspect ratios cast new light on some novel phenomena such as photomechanical effects, shape memory and excess scattering in molecular, polymeric and liquid-crystal glassy systems, where local orientationally ordered domains play an important role.

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Glassy Dynamics in Two-dimensional Melting

Huaguang Wang, **Zexin Zhang** (Soochow Univ.)

The nature of two-dimensional (2D) melting is an important topic in condensed matter physics research. Despite half of century of intensive research, there is still no universal theory to explain 2D melting. Over the years, computer simulations and experiments have confirmed the predictions made by the KTHNY theory that 2D solid melts from crystal to an intermediate hexatic phase, and then from hexatic to liquid. Previous work primarily focused on the static structure and order parameter evolutions during 2D melting, while dynamics receive much less attention. Herein, we study glassy dynamics and dynamical heterogeneities during 2D melting by colloidal experiments and computer simulations. Firstly, we observe an intermediate hexatic phase and exponential decay of orientational correlation, which are in excellent agreement with the KTHNY theory. More importantly, we found that the hexatic phase exhibits strong dynamical heterogeneity, showing a non-monotonic trend verse density/temperature. Interestingly, string-like structures of particles moving cooperatively are observed in hexatic phase. It is well known that the string-like structures are dynamical signatures of glass-forming liquids according to the classical Adam-Gibbs's glass transition theory. Thus, our studies provide unique perspectives on studying glassy dynamics.

Key Words: Glass, 2D melting, Structure, Dynamics, Dynamical Heterogeneity

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Inter-diffusion and self-diffusion in liquid Ce80Ni20

Bo Zhang (HFUT)

The inter-diffusion coefficients of Ce-Ni were measured in liquid Ce80Ni20 alloys by sliding cell method. The results indicate that the inter-diffusion strongly deviated from the standard Darken prediction and the relationship between inter-diffusion and self-diffusion should be described by the Darken–Manning equation. The dynamical cross correlation factor S of this liquid alloys is in the range of 0.6~0.8, which is much different from the solid where the S factor is always lager than 1. The linear response theory shows that the dynamical cross correlation factor is closely related with the distinct diffusion coefficients, or rather the deviation parts of the distinct diffusion coefficients to the reference diffusion system. In Ce80Ni20 melts, the abnormally small S was directly originated from the enhanced Ce-Ni distinct diffusion and reduced Ni-Ni distinct diffusion. The different mixing and movement tendency of dynamical behaviors in real liquid diffusion system is largely due to the "chemical" interactions among atoms. In the Ce80Ni20 alloy melts, the heterogeneity of dynamics caused by the chemical interactions makes the distinct diffusion of Ce-Ni and Ni-Ni deviate from the ideal diffusion behaviors, and finally leads to the failure of the Darken formula.

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Hu, J. L., Zhong, L. X., Zhu, C. A., Zhang, B., Inter-diffusion and its correlation with dynamical cross correlation in liquid Ce80Ni20, Appl. Phys. A. 123, 176 (2017).

Glass Transition of Polymer in Nanochannels

Xiaohua Zhang (Soochow Univ.), Zhaohui Yang, Jiadong Sheng

The glass transition behavior of polymer in a confinement has been a fascinating topic in the polymer physics society. We studied the glass transition behavior of polymer confined in the intertube channels of carbon nanotubes (CNT) using differential scanning calorimetry. The influence of nanochannel size on glass transition behavior was investigated. The glass transition temperature of polystyrene confined in the intertube channels of CNTs is suppressed as compared to its corresponding value of bulk sample. The effects of polymer molecular weight on the glass transition behavior are also investigated. We believe our study might provide a new understanding for the glass transition behavior of confined polymers.

Complex Structures and Dynamics Resulted from Long-range Anisotropic Interactions

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Repeating of isotropic building blocks produces ordered arrays with simple crystalline symmetry. In contrast, adding shapes to isotropic ones brings complex geometric tiling and repeating structure unites, yielding extension of simple crystalline structure to superlattices, quasicrystals or dynamically arrested amorphous structures. Matching between geometric tiling also generates different type of modes of structure relaxation, greatly affects mechanical properties such as ductility, plasticity, fragility, friction and lubrication in solids. However, in the structure organization process, both nearby geometric confinements between building blocks and far away extended anisotropic potentials take effects, therefore thermal dynamics and kinetics both run in a complicated way. In this study, we tackle this issue with 2D granular solids of shaped magnetic particles, which can extend their anisotropy through repulsions over a wide range. From isotropic disk, we systematically break the rotational symmetry of particles to square and triangular, probe their affection on bulk symmetry and relaxation kinetics. Over a broad density range, the square and triangular symmetry of particles do not break the quasi-long ranged 6-fold bulk symmetry of particle centers. Interestingly, breaking rotational symmetry of particles distinctively changes vertices structures of the two systems. Bulk symmetry of vertices structures is six-fold medium ranged in square-particles systems, but are characterized by small amount of dodecagonal edges. Breaking rotational symmetry of particles also changes the relaxation kinetics. Although relaxation are governed by dislocation dynamics, in square-particle systems, the kinetics are dislocation gliding, but in triangular-particle systems, the dislocation dynamics is governed by dislocation climbing associated with excitations along dodecagonal edges.

Key Words: Shaped particles, potential anisotropy, symmetry breaking.

Fracture mechanisms and strength theory of metallic glasses

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Owing to the unique amorphous structure, metallic glasses (MGs) exhibit quite distinctive deformation and fracture behaviors from the conventional crystalline materials. The high strength, brittleness and macroscopic homogenous and isotropic structural features make MGs ideal model materials for the investigations of the strength theory of high-strength materials. Hence the fracture behavior and strength theory of MGs have attracted very extensive interests of researchers from the fields of materials, mechanics and physics. This presentation is based on our research works on the fracture and strength of MGs in the past decade, and concentrates on discussing the current knowledge and recent advances on the fracture behavior and strength theory of ductile and brittle MGs, including some crystalline materials for comparision. At last, some unsolved issues associated with the fracture and strength of MGs are proposed.

KEY WORDS Metallic glass; yielding; fracture; deformation; strength theory

Mechanical properties of glasses: Rearrangement statistics and measures of ductility

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Amorphous materials such as metallic, polymeric, and colloidal glasses, exhibit complex preparation-dependent mechanical response to applied shear. In particular, glassy solids yield, with a mechanical response that transitions from elastic to plastic, with increasing shear strain. We perform numerical simulations to investigate the mechanical response of binary Lennard-Jones glasses undergoing athermal, quasistatic pure shear as a function of the cooling rate R used to prepare them. The ensemble-averaged stress versus strain curve $\sigma(\gamma)$ resembles the spatial average in the large size limit, which appears smooth and displays a putative elastic regime at small strains, a yielding-related peak in stress at intermediate strain, and a plastic flow regime at large strains. In contrast, for each glass configuration in the ensemble, the stress-strain curve $\sigma(\gamma)$ consists of many short nearly linear segments that are punctuated by particle-rearrangement-induced rapid stress drops. To explain the nonlinearity of $\sigma(\gamma)$, we quantify the shape of the small stress-strain segments and the frequency and size of the stress drops in each glass configuration. We decompose the stress loss (i.e., the deviation in the slope of $\sigma(\gamma)$ from that at $\sigma(0)$) into the loss from particle rearrangements and the loss from softening (i.e., the reduction of the slopes of the linear segments in $\sigma(\gamma)$), and then compare the two contributions as a function of R and γ. For the current studies, the rearrangement-induced stress loss is larger than the softening-induced stress loss, however, softening stress losses increase with decreasing cooling rate. We characterize the structure of the potential energy landscape along the strain direction for glasses prepared with different R, and observe a dramatic change of the properties of the landscape near the yielding transition. We then show that the rearrangement-induced energy loss per strain can serve as an order parameter for the yielding transition, which sharpens for slow cooling rates and in the large system-size limit. Finally, we investigate measures of the ductility of glasses prepared at different cooling rates and using different atomic interaction potentials. We show that glasses with a large accumulation of stress drops in the putative elastic regime are more ductile than glasses that do

not undergo such stress drops.

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