

tion structure and the dislocation annihilation process would predominate. The critical condition of the formation of dislocation jamming is studied and the intrinsic effect for crystal plasticity is revealed.

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14:20—Function Hall C

Self-healing of GaAs nanowires: an atomistic study

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Fractured GaAs nanowires (NWs) with a zinc-blende structure can spontaneously self-heal throughout Ga-As re-bonding at fracture sites. In this paper, a systematic molecular dynamics study has been made with focus on the influence of lateral dimensions of GaAs NWs, multiple fractures and atomistic diffusion on the self-healing process. The results show that, as the lateral dimension increases from 2.31 to 9.23 nm, GaAs NWs lose their 46.0% capacity of self-healing. After 24 repeated cycles of fracture, the restored tensile strength of a NW reduces by 64.4%. Atomistic diffusion enhances the healing efficiency by eliminating mismatch of atoms.

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14:40—Function Hall C

Multiscale modeling of multi-physics

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In this paper, the concern is the design and manufacture of synthetic and hierarchical material systems in which organization is designed and controlled on length scales ranging from nanoscopic to microscopic, even to macroscopic. Molecular dynamics (MD) and continuum mechanics are two distinct fields, very mature and successful in its own right. However, continuum mechanics is invalid for material systems at nanoscale and, even with a state-of-the-art supercomputer, MD is limited in the length/time scale that it can handle. Not only the difference in length scales is enormous, the concepts behind continuum theory and atomistic

theory are different like day and night. Therefore bridging the gap between MD and continuum mechanics theoretically and numerically has become imperative and remains as a grand challenge. Here we present a multiple-length/time-scale formulation of coarse-grained non-equilibrium molecular dynamics simulation.

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15:00—Function Hall C

Intrinsic lengths govern failure mode transition in metallic glasses

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It was reported that a switch from highly inhomogeneous to fully homogeneous deformation occurs when the sample size is small enough, from the tests on micropillars of metallic glasses (MGs). This suggests that the deformation in MGs is strongly size-dependent. However, what sizes controlling the mode transition remains unclear. In this paper, two intrinsic lengths a_{cI} and a_{cII} are proposed, respectively relating to the size of shear transformation zones and the sample dimension. Homogeneous deformation, intermittent shear banding and highly localization can be characterized by these two lengths. Furthermore, it is found that the two length scales measure the macro-plasticity of MGs and reveal the mechanism underlying the size effect of plasticity.

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15:20—Function Hall C

Nanostructured networks: materials and applications

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Networked materials, from buckypapers to cytoskeletons, feature structural hierarchies from nano to macro. With the combination of cutting-edge nano-engineering techniques and novel inspiration from biology, synthetic networked materials hold great potential in a number of applications, e.g., active, responsive, dynamic materials. In addition to the detailed properties of building blocks, interfaces and network topology, emergent phenomena also present. In this talk, we first present an analysis on the basic structural and mechanical properties of simple networks, followed by discussion on the structures, properties and transport behavior of several networked materials, including networks of carbon nanotubes, graphene and cytoskeletons. Specific focus will be placed on their applications in sustainable energy and environmental industry.

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