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臺灣大學應用力學研究所
演 講 公 告

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主 講 人：羅友杰 副教授
國立陽明交通大學 材料科學與工程系

講　　題：介觀動力學蒙地卡羅方法探討塊狀金屬玻璃與奈米玻璃之剪切局域化行為

摘　　要： 如附件

主 持 人： 張建成教授

時　　間： 114年12月01日（星期一）下午2時20分開始

地　　點： 臺灣大學應用力學研究所國際會議廳

☆☆ 歡迎聽講，敬請張貼 ☆☆

介觀動力學蒙地卡羅方法探討塊狀金屬玻璃與奈米玻璃之剪切局域化行為

Mesoscale Kinetic Monte Carlo Modeling of Shear Localization in Bulk Metallic Glasses and Nanoglasses

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Abstract

Shear localization in metallic glasses (MGs) critically limits their mechanical performance. Bulk metallic glasses (BMGs) typically deform via highly localized shear bands, often exhibiting serrated flow, while nanoglasses (NGs), composed of glassy grains connected by softer interfaces, offer a promising strategy to mitigate catastrophic failure. In this work, we integrate in situ thermal imaging experiments and mesoscale kinetic Monte Carlo (kMC) simulations to elucidate the spatiotemporal evolution of shear bands in BMGs and NGs. For BMGs, synchronized correlations between stress drops and transient heat bursts reveal that serrations originate from coupled structural and thermal softening during shear band nucleation and reactivation. A modified kMC model incorporating heat diffusion successfully reproduces this behavior. For NGs, we develop a novel mesoscale kMC framework with a variable characteristic strain (VCS) to capture grain size effects. Simulations reveal a transition from inhomogeneous to homogeneous deformation as grain size decreases to ~10 nm, where interfaces guide early shear transformation zone (STZ) activities and hinder the formation of dominant shear bands. Progressive reduction of elastic constants further reproduces experimentally observed brittle-to-ductile transitions. The combined findings provide a unified, multi-scale understanding of shear localization mechanisms in amorphous alloys and offer design guidelines for tailoring NG microstructures to enhance shear resistance.