MS06: Effects of small size scales in materials modeling
16:00–18:00, Monday, 20 August
Bill Curtin, Switzerland, Chair
Baohua Ji, China, Chair
Room: Function Hall C

16:00–Function Hall C

Twin boundary: strengthening or softening?

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Coherent twin boundary is a special kind of internal interface with low energy. It can serve as sink and source of dislocations, as well as barrier against dislocation transmission, which is regarded as effective strengthening internal interface for most materials. An increase in twin density with decreasing twin thickness can strengthen ultrafine-grained Cu, similar to the grain-size-dependent strengthening in nanocrystalline metals. In this presentation, we will focus on the recent studies not only of the strengthening but also of the softening phenomena relative to the coherent twin boundaries. The effect of ultra-fine twin thickness, temperature as well as loading orientation on the strength, ductility and work hardening of Cu with nano-scale twins will be reported. A novel partial dislocation nucleation governed plastic deformation mechanism is responsible for the de-twinning and softening of metals with nanoscale twins. The softening deformation will eventually advance the understanding the plastics deformation mechanism of nanotwinned metals.

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16:20–Function Hall C

A quasicontinuum approach to modeling discrete microstructures

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The quasicontinuum method, which was developed for atomic lattices, is extended to a more general class of microstructural models in which discrete points interact via discrete interactions. Such models allow one to study the influence of small-scale features (e.g., defects) in large-scale problems in a natural fashion, but may be prohibitively expensive. The quasicontinuum method allows one to reduce the resolution of the description where appropriate, so that realistic simulations become feasible. It is entirely computationally based and makes use only of the underlying discrete microstructural model. In order to render the method applicable to a much wider class of problems than atomistics, the conventional energy based method is reformulated in terms of a virtual power balance. The summation rules used to account for the influence of discarded lattice points are also revisited. The performance of the resulting method is illustrated by an example in which the lattice points are connected by elastoplastic trusses.

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16:40–Function Hall C

Some observations on the size effects in nanotwined metals and their theoretical explanation

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When materials are deformed plastically via dislocations, a general finding is that samples with smaller dimensions exhibit higher strengths but with very limited amount of plasticity in tension. Here we report that one-dimensional coherent nanostructures with tilted internal twins exhibit anisotropic size-effect: their strengths show no apparent change if only their thicknesses reduce, but become stronger as the sample sizes are reduced proportionally. Large-scale molecular dynamics simulations show that such NWs deform primarily through twin migration mediated by partial dislocations in one active slip system, and a large amount of plasticity could be achieved in such nanowires via twin migration. The unique structure shown here is suitable to explore strengthening mechanisms in metals when plasticity is controlled by a single dislocation slip system. This study also suggests a novel approach to modulate strength and ductility in one-dimensional coherent nanostructures.

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17:00–Function Hall C

Atomistic investigation of enhanced tensile ductility of metallic glass matrix composite with crystalline second phase

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The concept of Metallic glasses (MG) matrix composites (MGMCs) has been raised to achieve optimized mechanical properties, especially improved tensile ductility. In general, the composite is composed of a crystalline second phase embedded in a MG matrix. It remains difficult to capture shear band evolution in experiments and thus impossible to correlate the measured mechanical properties with discrete plastic events at small length scales. It is thus worthwhile to conduct atomistic simulations to gain further insights into the deformation mechanisms of MGMCs. We show that, by designing patterns of nanocrystals in MGMCs, shear bands in the MG matrix can be arrested at crystal/glass interfaces. Though mechanisms of shear band branching, reflection, and penetration though crystals, a shear band network is finally formed in the highly deformed MGMC structure. It is observed that the propagation of a few major shear bands, which is the reason for fracture in pure BMGs, is greatly suppressed.

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