the results of the Kolmogorov-Arnold-Moser theory. All the resonances of up to fourth order inclusive encountered here are listed and studied. The investigations of Havelock who solved this problem in a linear formulation are thereby completed.

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14:51–Function Hall C

Theoretical relations between quantities at a water surface and the instantaneous subsurface flowfield

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We consider theoretical aspects of estimating the instantaneous subsurface flow field based on measured distributions of velocity, and possibly water level, over the surface of a river or sea, with allowance for a river bank (seabed). Considering incompressible kinematics first, an integral relation is derived that relates surface velocities to the subsurface vorticity field. Then dynamical relations that involve total head at the surface, which would additionally require measured distributions of fluctuating surface height, are similarly derived.

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MS06: Effects of small size scales in materials modeling
16:10–18:10, Tuesday, 21 August
Yong-Wei Zhang, Singapore, Chair
Quanshui Zheng, China, Chair
Room: Function Hall C

16:10–Function Hall C

Discrete dislocation analyses of size effects in plasticity

A. Amine Benzerga[†], *Shyam M. Keralavarma, P.J. Guruprasad*
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We analyze plasticity size effects by means of computational discrete dislocation dynamics. We consider loading situations in compression and bending immune of the kind of artefacts encountered in experimental nanomechanics experiments. Using an enhanced method capable of simulating hardening and millions of interacting dislocations, we explore behavior transitions under compression in the space of meaningful structural parameters and discuss the relevance of our predictions to micropillar experiments. In the high dislocation density regime we offer an explanation of size dependent hardening on the basis of an evolving dislocation substructure monitored in terms of GNDs. We also analyze the plastic response in pure bending and the contribution of GNDs to dissipation versus energy storage as the size of the bent crystals approaches the micron.

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16:30–Function Hall C

Understanding the size effect in the mechanical properties of nanotwinned copper

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We performed large-scale molecular dynamics simulations to study the plastic deformation of nanotwinned polycrystalline copper. Our simulations showed that the materials' plastic deformation was initiated by partial dislocation nucleations at grain boundary triple junctions. Although both dislocation cutting across twin boundaries and dislocation-induced twin migrations were observed, our quantitative analysis revealed that the cutting interaction through a Lomer dislocation mechanism was the dominant one. We further examined the effect of twin spacing on this dominant mechanism through a series of specifically-designed nanotwinned copper samples over a wide range of twin spacing. The simulations showed that a transition in the dominant deformation mechanism occurred at a small critical twin spacing. Based on these observations, a simple, analytical model for the critical twin spacing was proposed and the predicted critical twin spacing was shown to be in excellent agreement both with respect to the atomistic simulations and experimental observation.

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16:50–Function Hall C

EEffect of vacancies on the ultimate tensile strain of ZnO nanowires

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Some of experimental measurements show significant size effects on Young's modulus and strength of ZnO nanowires (NWs), while others do not. To address this paradox, influences of lateral dimension and vacancy on the tensile behavior of ZnO NWs are assessed using molecular dynamics simulations. The results for defect-free NWs show that the ultimate tensile strain (UTS) of wurtzite structure varies 6.7% as lateral dimension increases from 2.93 to 5.53 nm. However, behaviours of ZnO NWs with vacancies reveal that vacancies can significantly reduce the UTS by 43%, which is comparable to the range of data scatter, about 50%, observed in experiments. The influence of the positions of vacancies is also discussed. This work provides a better understanding on the large scatter of UTS observed in experiments.

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