NOMATEN JUNIOR SEMINAR

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Dislocations and nanomechanics in alumina using atomistic simulations

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Abstract:

The study of nano-objects is of particular interest due to their outstanding mechanical properties. While metal nanocrystals are generally characterized by high yield strength and ductility under extreme compressive stress, very few is known about other classes of materials including ceramic or semi-conductors. Recently, it was shown that ceramic nano-particles such as aluminum or magnesium oxides could plastically deform under high stress without cracking what might have significant implications for the sintering and compaction of nanocrystalline ceramics. However, only few evidences of the elementary deformation processes were addressed so far, especially in the case of α-Al2O3 nanocrystals.

In this study, we propose to investigate α-Al2O3 nanoparticle mechanics using molecular dynamics simulations. Firstly, several α-Al2O3 bulk properties as lattice and elastic constants, stacking-fault and surface energies as well as basal edge dislocation features as compared to existing experimental/numerical literature are investigated to test the transferability of various interatomic force fields to the nanomechanical field. Among all the tested parameterizations, the 2/3-body Vashishta interatomic potential has shown to be particularly adapted to the overall study. Secondly, nanoparticle compression tests are modeled as function of orientation and temperature including a detailed analysis of dislocation-based mechanisms for several sizes of α-Al2O3 nanoparticles. Results are discussed in the context of recent nanomechanics experiments as well as pioneer works performed on bulk alumina.

Bio:

Qinqin Xu had earnd his Doctor degree at the MATEIS lab, INSA de lyon, French. His project was funded by the Chinese Scholarship Council (CSC). Recently he is emlpoyed as assistant professor at NOMATEN Centre of Excellence at the National Centre for Nuclear Research, Poland.