Symposium | A. Advances in Materials Theory for Multiscale Modeling

## [SY-A1]Symposium A-1

Chair: Anton Van der Ven(University of California Santa Barbara, United States of America)
Mon. Oct 29, 2018 1:30 PM - 3:00 PM Room6

# [SY-A1]Finite-temperature Localized Stress and Strain for Atomic Models

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Homogeneous deformation of an ordered crystalline solid at finite temperature can cause non-affine transformation of atomic trajectories, particularly when the inter-atomic potential is anharmonic. In such a case, continuum measures based on affine transformation of trajectories are insufficient to ensure energetic equivalence between the atomic and continuum scales and non-classical stress measures are required. These measures also need to be localizable to obtain continuum stress and strain spatially resolvable to atomistic scales. To this end, the total work done on an atom under deformation is decomposed into the work corresponding to changing its equilibrium position and work corresponding to changing its second moment about equilibrium position. Correspondingly, we define two kinematic variables: a deformation gradient tensor and a vibration tensor, and derive their stress conjugates, termed here as static and vibration stresses, respectively. The proposed approach is validated using MD simulation in NVT ensembles for fcc aluminum subjected to uniaxial strain at high temperatures up to 0.9Tm. Highly non-linear and non-affine evolution of second moments are observed in the elastic portion of the high temperature-high tensile strain regime, in which the conjugate pair of vibration stress and vibration tensor contribute significantly to free energy change, particularly as the material approaches elastic instability through violation of the Cauchy-Born rule. In the elastic portion of the compressive regime, the non-affinity of the second moments point to anomalous phonon dispersion and non-monotonic variation of average group velocities with strain, which resembles experimental observations in certain crystalline solids. The results are strongly relevant for developing finite temperature continuum theories based on discrete simulations or inter-atomic potentials.