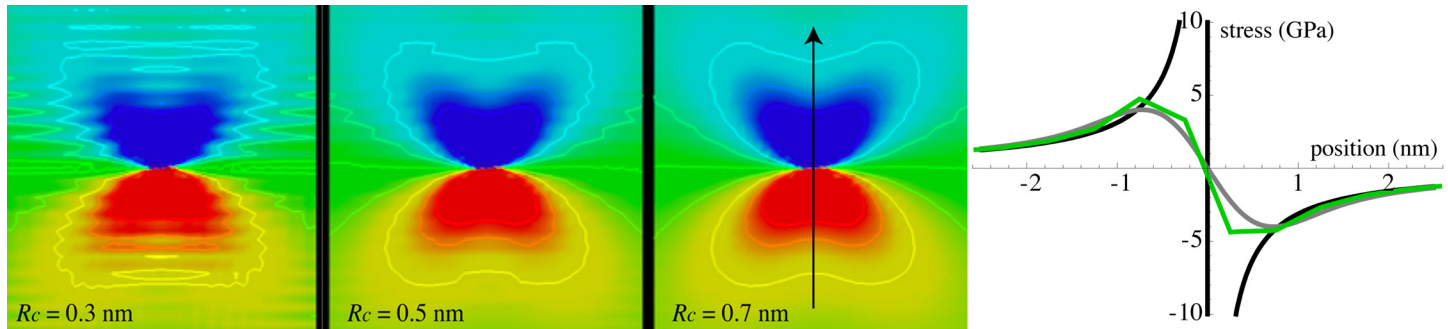




# Materials Science and Technology

## Nanomechanics

# Atomic Simulation Guides Nanomechanics Theory



**Figure 1:** Left: Stress field around a dislocation core showing regions of compressed (blue) and stretched (red) crystal. As the spatial averaging volume size is increased from 0.3 to 0.7 nm, contours of constant stress become more continuous. Right: Stress as a function of position along the line shown for a 0.7 nm averaging volume. Local elasticity theory (black) fails to properly describe stress within a 2 nm region surrounding the defect while non-local elasticity (grey) – fit to atomistic simulation (green) – does.

*Nanoscale stresses at defects require new theoretical approaches*

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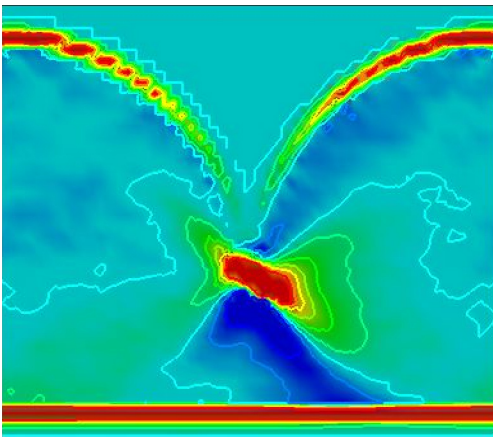
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Continuum theory has been used for decades to analyze and predict the mechanics of materials and structures as diverse as airplanes to prosthetics. However, as existing and emergent technologies shrink to the nanometer range, quantities such as stress and strain become ill defined and the application of continuum mechanics in nanomechanical frameworks becomes suspect. Manufacturing implications are significant; for example, traditional design tools do not accurately apply to microscale or nanoscale electro-mechanical systems because continuum mechanics concepts, on which those design tools are based, do not apply on such length scales. While modeling and simulation methods (e.g., molecular dynamics) have provided a wealth of information for such systems, connections to engineering scale analysis are not clear.

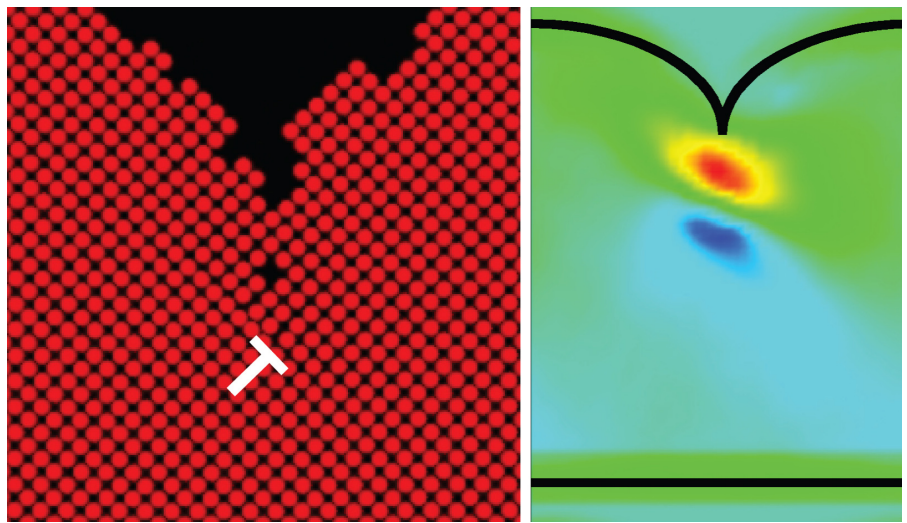
Researchers at Sandia have been investigating and refining definitions for continuum variables at the atomic scale. The result is that quantities inherent to atomistic simulation, such as atom positions, velocities and inter-atomic forces, can be used to determine spatially varying stress fields. These definitions effectively overlay a continuum representation on an atomistic

system. Weighted spatial averages of atom quantities within finite-sized volumes are used to estimate stress at the material points corresponding to those volumes. Time averaging these estimates permits meaningful comparison to continuum theory. For example, analysis of an edge dislocation in a crystal (an imperfection in the local ordering of the crystal's structure) reveals that averaging volumes surrounding continuum material points must be of a minimum dimension (~0.7 to 1.0 nm) in order for stress fields to be resolved in a continuous fashion (Fig. 1). This analysis also shows that variation of stress close to the dislocation core (or center) is not well represented by conventional local elasticity theory, but rather by more advanced non-local theory. Most significantly, marrying non-local elasticity theory to atomistic simulation permits direct determination of length scale parameters that achieve accurate description of the stress surrounding the material defect. Thus, atomistic simulation employing newly defined mechanics variables can be used to develop robust nanomechanics theory.

Atomistic-based expressions for stress were used to gain fundamental understanding of materials behavior:



**Figure 2:** Results from a molecular dynamics simulation are used to predict the stress field during the initial coalescence of growing islands (a two dimensional cross-section is shown from a three dimensional simulation). Tensile stress (red) is concentrated within the coalescence region, signifying the formation of a dislocation defect. Also discernable is tensile stress that occurs at the island surfaces, tensile stress near the substrate's bottom free surface and compressive stress (blue) that exists within a majority of the volume of the islands (due partly to surface curvature effects).



**Figure 3:** Results from a molecular dynamics simulation are used to show the formation of a defect (left) and the evolution of stress (right) that occurs during ongoing coalescence of islands in a growing film (two dimensional cross-sections from three dimensional simulations are shown). For clarity, a white 'T' is placed at the location where the defect is formed while black lines show the approximate locations of the islands' free surfaces and the substrate's bottom free surface.

specifically, stress evolution during metallic thin film growth. During such growth, isolated islands are first nucleated, and then proceed to coalesce and form continuous planar films. While experiments have successfully quantified the average stress within a film during growth, little is known about the distribution of stress within a film or whether defects form as island coalescence occurs. Molecular dynamics simulations confirmed suppositions from experiment that coalescence happens in two stages: initial coalescence occurs when neighboring islands first join together. At that point a dislocation defect is formed and a concentration of tensile stress exists within the coalescence region (Fig. 2). After initial coalescence, ongoing coalescence is exhibited and new defects are periodically formed. While this ongoing coalescence stage reduces system energy through the elimination of surfaces, tensile stress continues to increase during defect formation events (Fig. 3). Such nano-mechanical analysis can provide guidance on choosing growth conditions that lead to films of specific morphology and structure.

## References:

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