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# NANO HIGHLIGHT
# Atomistic Characterization of the Influence of Pre-Existing Stress on the Interpretation of Nanoindentation Data: Universal Behavior Across Length Scales

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We have accurately determined the true contact area during plastic indentation of materials under an applied in-plane stress using atomic-level simulations. We find that the mean pressure calculated from true contact areas, which take into account plastic pile-up around the indenter, varies only slightly with applied pre-stress, with higher values in compression than in tension, and that the modulus calculated from the true contact area is essentially independent of the pre-stress level in the substrate. On the other hand, if the contact area is estimated from approximate elastic formulae often assumed in experimental indentation studies, the contact area is under estimated, leading to a strong, incorrect dependence of apparent modulus on the pre-stress level. Our simulations demonstrate that this phenomena, namely an apparent incorrect dependence of mechanical properties on initial stress state, first reported for macro-scale hardness measurements dating back to 1932, also exists at the nanometer-scale contact areas, apparently scaling over 10 orders of magnitude in contact area, from ~mm$^2$ to ~100nm$^2$.

Indentation as a means to determine materials properties has a long and rich history dating back to Hertz and Boussinesq, who in the 1880's developed methods for computing the stresses and displacements for contacting elastic bodies. Starting in about 1900, Brinnell investigated indentation of metals by large spherical indenters (macroindentation), and showed that a material's resistance to indentation, also known as hardness, is a good measure of the steel's resistance to mechanical deformation. Over the last two decades nanoindentation, a method in which continuous load-displacement curves are measured with nanometer-scale resolution, has been increasingly used to characterize materials properties with depth and spatial resolutions that are comparable to key scales in new nanotechnologies, including feature sizes of current relevance to the microelectronics industries. Properly interpreting these curves, however, is crucial to using this probe of mechanical properties for nanofeatured systems, as our simulations described above have clearly shown.

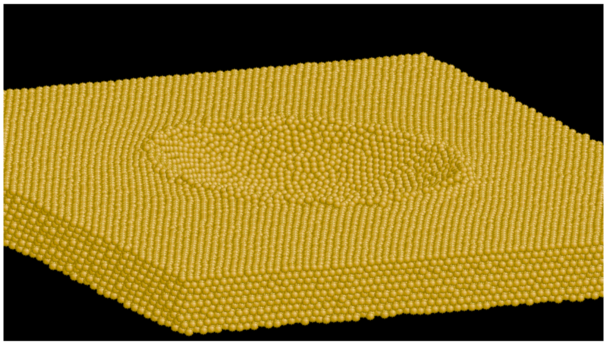

FIG1 : Illustration of the contact area around a simulated nanoindentation. Each sphere represents an atom. An initial region of "pile-up" around the indenter due to plastic deformation is apparent.

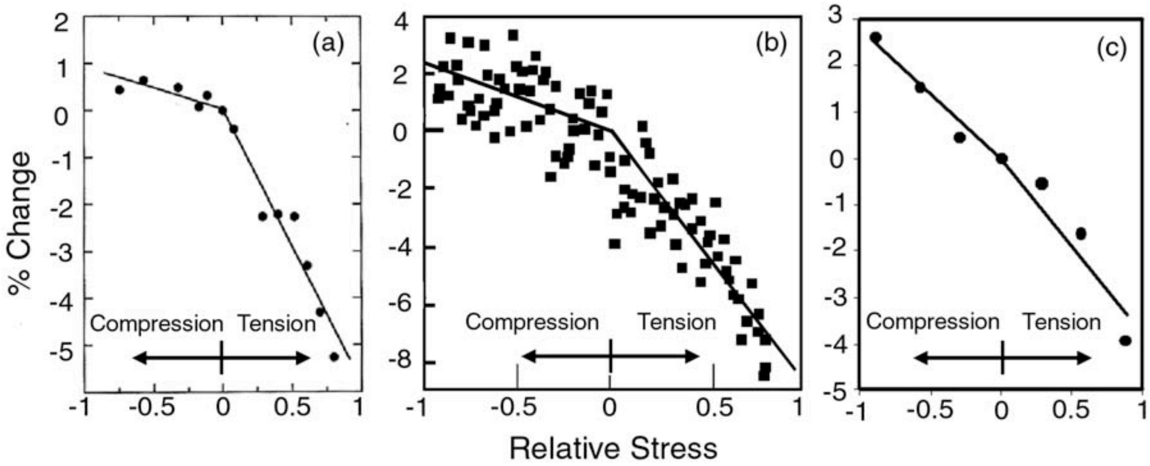

FIG 2. Changes in hardness/modulus as a function of scaled in-plane stress for three regimes of contact area. The changes with stress are a result of the use of approximate elastic formulae to calculate contact areas and do not reflect real changes in materials properties. (a) **mm$^2$ scale**: Rockwell B hardness data for high-carbon steel, (from G. Sines and R. Carlson, ASTM Bulletin **180**, 35 (1952)). (b) **_m$^2$ scale**: Modulus data for an aluminum alloy (reproduced from.Y. Tsui, W.C. Oliver and G.M. Pharr, J. Mater. Res. **11**, 752 (1996)). (c) **nm$^2$ scale**: Relative modulus obtained by our simulated plastic nanoindentation of gold.

**Reference**: J.D. Schall and D.W. Brenner, “Atomistic simulation of the influence of pre-existing stress on the interpretation of nanoindentation data”, J. Mat. Res., submitted.