Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

A Servo-Controlled Atomic Break Junction: Closing the Gap between Experiment and Modeling DOUGLAS SMITH, JON PRATT, FRANCESCA TAVAZZA, NIST — Measurement of force and displacement in atomic-scale deformation experiments enables direct measurement of atomic bond strength and stiffness, promises insight into phenomena like adhesion and friction, and promises to provide reliable experimental data for atomistic models. Such experiments require displacement accuracy well below atomic dimensions and force accuracy below predicted atomic-bond rupture forces of 1.5 nN. A break junction instrument has been realized that uses a fiber-optic laser interferometer to hold the position of a gold contact stable to better than 5 pm for tens of minutes in vacuum at 4 K. This has allowed a careful study of quantized electron transport through a gold junction as it is drawn down to a single Au-Au bond and broken. Density functional calculations show that the junction necks down to a single bond that breaks with a reproducible rupture force that is independent of the crystallographic orientation of the original junction. The work represents one of the first direct deformation studies of an experimental system small enough to be modeled in its entirety using density functional methods.

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Date submitted: 20 Nov 2008 Electronic form version 1.4