

Breakdown of a Au nanowire between electrodes

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Structural properties of junctions made of an atomic Au wire placed between Au electrodes, were investigated using the method of linear muffin-tin orbitals (LMTO) within the local-density approximation (LDA). We studied the dynamical motion of the atoms in the wire. A soft phonon mode was found. Large displacements which resulted in wire breakage was also studied. The energy barrier associated with this junction-break process has been compared with some experimental results. This work was supported by NSF grant ECS0304682.

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