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Local and global instabilities in nanosize rectangular prismatic gold specimens

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ABSTRACT

We use molecular mechanics simulations with the tight-binding potential to study local and global instabilities in initially defect-free nanosize rectangular prismatic specimens of gold deformed in tension/compression and simple tension/compression. Whereas in simple tension/compression atoms on end faces are constrained to move axially but are free to move laterally and the cross-sectional dimensions of end faces can change, in tension/compression all three components of displacements of atoms on end faces are prescribed and the cross-section of an end face does not change. The three criteria used to delineate local instabilities in a specimen are: (i) a component of second-order spatial partial derivatives of the displacement field has large value relative to its average value in the body, (ii) the minimum eigenvalue of the Hessian of the potential energy of an atom is negative, (iii) a relatively high value of the common neighborhood parameter. A specimen becomes globally unstable when its potential energy decreases noticeably with a small increase in its deformations. It is found that the three criteria for local instability are met essentially simultaneously at the same atomic position. Deformations of interior points of a specimen are different when it is deformed in simple tension/compression from those in tension/compression. It is found that the initial unloaded configuration (or the reference configuration) of the minimum potential energy has significant in-plane stresses on the bounding surfaces and non-zero normal stresses at interior points. This initial stress distribution satisfies Cauchy's equilibrium equations for a continuum. In deformations of a nanobar studied here, the yield stress defined as the average axial stress when the average axial stress vs. the average axial strain curve exhibits a sharp discontinuity depends upon the specimen size. It is shown possibly for the first time that deformations of the specimen are reversible if it is unloaded prior to yielding but have a permanent strain if unloaded after it has yielded. Because of residual stresses in the reference configuration, the average axial stress at yield in compression is nearly one-half of that in tension. The slope of the average axial stress vs. the average axial strain curve during unloading after it has yielded is the same as that during initial loading up to the yield point.

1. Introduction

Mechanical properties of materials with one or more dimensions of the order of nanometers are of great interest due to the potential use of nanosize specimens as reinforcements in fabricating composites for structural applications and in the development of electrical, thermal and optical systems. Materials at the nanoscale have special features related mostly with the prominent influence of stresses induced in free surfaces and the residual stresses developed in the interior of the body.

The influence of surface and residual stresses can be important on the mechanical properties of a nanostructure. With a decrease in cross-sectional dimensions of a nanowire the interatomic spacing between atoms near the free surfaces decreases from that in a perfect crystal. The variation in the interatomic forces develops stresses in the specimen that may affect its response to subsequent loads. It has been observed in molecular mechanics/molecular dynamics (MM/MD) simulations that in-plane tensile stresses on the bounding surfaces generate compressive normal stresses in the interior of a nanowire [1,2].

Diao et al. [1] have used the modified embedded atom method (EAM) potential [3] to simulate tensile deformations of gold specimens of square cross-section oriented in the [1, 0, 0] and [1, 1, 1] crystallographic directions. They computed the effective Young's modulus E and Poisson's ratio ν for different cross-sectional areas. For 3 nm thick nanowires oriented in the [1, 0, 0] direction, E equaled 42.3 GPa. We note that E for the bulk gold material also equals 42.3 GPa. However, for nanowires less than 1.83 nm thick E increased to 127 GPa. The local virial stress tensor computed in the initial unloaded relaxed or the reference configuration gave in-plane tensile stresses in nanowire's bounding surfaces and compressive stresses in the interior. For 2 nm thick wires, values of E at the four corners of the cross-section were 3.5 times of those at

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interior points. For nanowires in the [1, 0, 0] direction, the magnitude of the compressive stress at an interior point exceeded 1.6 GPa which is the yield stress in compression for a bulk material.

Gall et al. [4] have studied the effect of free surfaces in rhombic and multishell nanowires. The rhombic nanowires had [1, 1, 0] axis orientation and {1, 1, 1} side surfaces while the multishell wires were composed of a single atomic chain surrounded by a helix of six atoms. MD simulations of tensile loading using the EAM potential were performed until yield signified by a sharp discontinuity in the average axial stress–average axial strain curve. Young's modulus of a multishell wire was found to be greater than that of a rhombic nanowire. For a 0.7 nm diameter multishell wire the average axial yield stress and the average axial yield strain were 13 GPa and 14%, respectively. For a 2.2 nm diameter rhombic nanowire the average axial yield stress and the average axial yield strain were 3 GPa and 7%, respectively. Gall et al. [4] explained that the {1, 1, 1} surfaces contract without the application of an external load generating compressive stresses in the interior of the wire. The effect of surface stresses is negligible for macroscopic bodies but is significant for specimens of diameter less than 10 nm. They pointed out that the initially compressive stresses cause the experimentally observed asymmetry in the yield stress for small diameter specimens deformed in tension and compression. In a tension test after the external loads have overcome the internal compressive stress the wire fails due to a tensile stress reaching a limiting value. Although free surfaces contribute to the generation of internal compressive stresses that increase the strength of the structure under tension, points with high compressive stresses and other geometric irregularities are potential sites for the nucleation of instabilities.

Diao et al. [5] studied the effect of free surfaces on the yielding of gold nanowires and proposed that points where the resolved shear stress reaches a critical value are unstable points, and dislocations nucleate there. Isothermal MD simulations at 2 K of tensile and compressive deformations of gold specimens of square cross-section with [1, 0, 0] and [1, 1, 1] axial orientation were performed using periodic boundary conditions in the length direction which equaled three times the thickness of the nanowire. For [1, 0, 0] nanowires less than 2.45 nm in thickness some material points in the reference configuration had yielded. With an increase in the axial strain imposed upon the reference configuration of the 4 nm thick nanowire oriented in the [1, 0, 0] direction, the average axial yield strain and the average axial yield stress equaled $\sim -4.8\%$ and ~ -0.7 GPa, respectively, in compression, and $\sim 10\%$ and ~ 4 GPa, respectively, in tension. For the same nanowire oriented in the [1, 1, 1] direction the average axial yield stress in tension and compression was ~ 5 GPa. The yielding was attributed to the nucleation and propagation of {1, 1, 1} [1, 1, 2] partial dislocations from edges of the nanowires. The Schmidt factor for a bulk material at the onset of yield for the most favorable slip system in the [1, 0, 0] nanowire is larger in compression than that in tension causing the [1, 0, 0] nanowire to yield at a lower value of the axial stress in compression than that in tension. However, the Schmidt factor for the most favorable slip system in the [1, 1, 1] nanowire is larger in tension than that in compression but the residual compressive stresses counteract this effect producing an equal value of the yield stress in tension and compression. Even though Diao et al. [5] found that the critical resolved shear stress does not change appreciably with the cross-sectional area of the nanowire and that it can be used as a criterion for the nucleation of defects, Liu et al. [6] and Miller and Rodney [7] have stated that the slip system with the highest resolved shear stress is not always activated at the yield point.

Zhang et al. [2] using the linear elasticity theory considered effects of the surface and the initial stresses to find analytical expressions for the effective Young's modulus, strains, stresses, and the yield stress in tension/compression for an isotropic nanowire with a circular cross-section and unit length. They found that the effective Young's modulus and, in general, elastic constants of the nanowire do not depend upon the residual stresses. Assuming the von Mises yield criterion, they derived an expression for the yield stress in tension and compression which showed that the initial stress is responsible for the asymmetry observed in the yield stress in tension and compression. It was also found that the influence of elastic properties of the surface and of the initial stresses on the effective elastic properties of a nanowire and on the yield stress diminish with an increase in the radius of the nanowire. It seems that the assumptions of the material being isotropic and residual stresses being uniform are not realistic for a nanowire.

In the quest for determining the strength of materials at small scales, an important problem is the investigation of the material instabilities and the failure of the structures under external loads. A possibility is to assume that a structural element has failed when stresses or strains at a material point have just reached the level to make its deformations inelastic and the material point cannot return to its original state upon complete unloading of the structure. In an atomic system, the onset of an irreversible deformation is termed instability. Although atomic systems are discrete continuum concepts have been used to characterize the onset of irreversible deformations [6,10,11,16].

In a homogeneous continuous body, a strong singularity is associated with either the deformation gradient or the displacement becoming discontinuous across a surface passing through a material point (e.g., see Truesdell and Noll [8]). The singularity is called weak when both displacements and their first-order spatial derivatives are continuous but a second or a higher-order spatial derivative of the displacement is discontinuous at one or more points of the body. The initiation of instability at a point is synonymous with an acceleration wave not propagating through that point [9]. This is equivalent to the acoustic tensor evaluated at that point having a zero eigenvalue or a null determinant. van Vliet et al. [10] and Steinmann et al. [11], amongst others, have used it to characterize local instabilities in an atomic system.

The hypothesis of the acoustic tensor becoming singular at the onset of a local instability is equivalent to assuming that the matrix of instantaneous values of elasticities, defined as the second-order derivatives of the strain energy density with respect to the Green-St. Venant strain tensor, ceases to be positive-definite. In the phonon theory the acoustic tensor is called the dynamical matrix and is a discrete quantity. However, in continuum mechanics the acoustic tensor is defined at every point in the continuum and is a continuous function of the deformation gradient. For discrete systems Lu and Zhang [12] have used an atomistic counterpart of the continuum acoustic tensor, called the atomic acoustic tensor, to study the nucleation of local instabilities. It is equivalent to requiring that the energy of every atom in the system in equilibrium be convex for variations of position vectors of other atoms given by a mono-mode perturbation.

Energy principles have also been applied to the study of the stability conditions in atomic structures. The configuration of a system in equilibrium is globally stable if its potential energy in that configuration is the minimum. Kitamura et al. [13] studied delamination of a nanofilm from a substrate and found that the displacement at which the minimum eigenvalue of the Hessian of the potential energy of the system vanished equaled that at which the load–displacement curve became discontinuous (the displacement abruptly increased with an small increase in the applied load). The same criterion has been used to analyze strengths of thin films and cracked bodies [14].

Instabilities in an atomic system have also been studied by the normal mode analysis [15] which exploits symmetries of the system to reduce the number of degrees of freedom (d.o.f.). For a