Vibrational Properties of Strained Gold Nanowires

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The purpose of this work is to study how the vibrational response of gold nanowires varies with axial stresses through classical molecular dynamics (MD) simulations. The considered nanowires are biclamped and have square cross-sections, where the axial and free surface normal directions correspond to \(\langle 100 \rangle\) crystallographic directions. Three different nanowire sizes were simulated: \(2.45 \times 2.45\) nm\(^2\), \(4.08 \times 4.08\) nm\(^2\), and \(5.71 \times 5.71\) nm\(^2\) cross sectional sizes, with the respective lengths \(29.4\) nm, \(49.0\) nm, \(68.5\) nm, which correspond to an aspect ratio of roughly 12. This ensures that the wires are slender and that elementary beam theory can be used for the continuum calculations [1]. The intermolecular interaction is modelled through an embedded atom method (EAM) potential, which has been exactly fitted to the elastic constants, the cohesive energy, the stacking fault energy, the vacancy formation energy and the lattice constant [2]. In order to excite unsymmetric modes, only half the nanowire was loaded transversally to ensure an unsymmetric deflection, from which the nanowire was released. The dynamic response was monitored and the eigenfrequency spectrum was obtained from a discrete Fourier transform of the dynamic history.

The continuum mechanical equation governing transverse free vibrations of an axially stressed beam can be derived from

\[
\frac{d^2}{dx^2} \left( EI \frac{d^2 w}{dx^2} \right) - \frac{d}{dx} \left( N_0 \frac{dw}{dx} \right) - \omega^2 mw = 0 \tag{1}
\]

cf. [1], where \(E, I, N_0, m,\) and \(\omega\) denote Young's modulus, the moment of inertia, the applied axial force, the mass per length unit and the angular eigenfrequency, respectively, and \(w\) denotes the deflection of the centreline. By imposing biclamped conditions, Eq. (1) can be solved numerically. For the analytical solutions of Eq. (1), it has been assumed that the linear elastic relation \(N_0 = AE\varepsilon\) holds, where \(A\) and \(\varepsilon\) denote the cross-sectional area and the axial strain of the nanowire.

A preliminary comparison between results from Eq. (1) and results from MD simulations can be seen in Figs. 1(a) - 1(c). Both results from wires in tension and compression have been compiled in 1(a) - 1(c). The increase in the fundamental eigenfrequency for highly compressed nanowires and the lowering of the fundamental eigenfrequency for nanowires that are significantly deformed in tension is due to the fact that they deform plastically. Comparing MD results with analytical results reveals that there is a good agreement for the larger sized nanowires, cf. Figs. 1(b) - 1(c). For the smallest nanowires, cf. Fig. 1(a) there are noticeable discrepancies between analytical and MD results, these discrepancies are particularly noticeable for small strains.

References


Figure 1: The fundamental eigenfrequencies for different amounts of strain for a) $2.45 \times 2.45 \, \text{nm}^2$, b) $4.08 \times 4.08 \, \text{nm}^2$, and c) $5.71 \times 5.71 \, \text{nm}^2$ cross sections. The solid line correspond to linear elastic solutions of Eq. (1).