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Article

A Multiple Site Type Nucleation Model and Its Application to the Probabilistic Strength of Pd Nanowires

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1. Finding the nucleation strain

The main point in measuring the nucleation strain is to identify a clear drop in tensile stress, which is characteristic of dislocation nucleation. We found that the following procedure yields the nucleation strain relatively precisely, and in a consistent manner between all simulations.

We first found the strain at which we reach maximum stress, as an indication of the approximate strain values at which dislocation is nucleated. Then, we fitted a parabolic function to the stress-strain curve, up to the strain at which the stress was maximal. Then, we looked for a range of strains, starting from the strain of maximum stress, in which the MD simulation results yielded smaller stresses than the parabolic fit. A range of strains of about 0.1% was found to be sufficient to identify a clear drop. If indeed the MD stress values were smaller than the fitted values, we choose the first strain value for which the MD stress was lower, to be the nucleation strain. We have found this automated procedure to determine rather accurately the nucleation strain in each simulation.

2. The energy barrier calculated using the nudged elastic band method

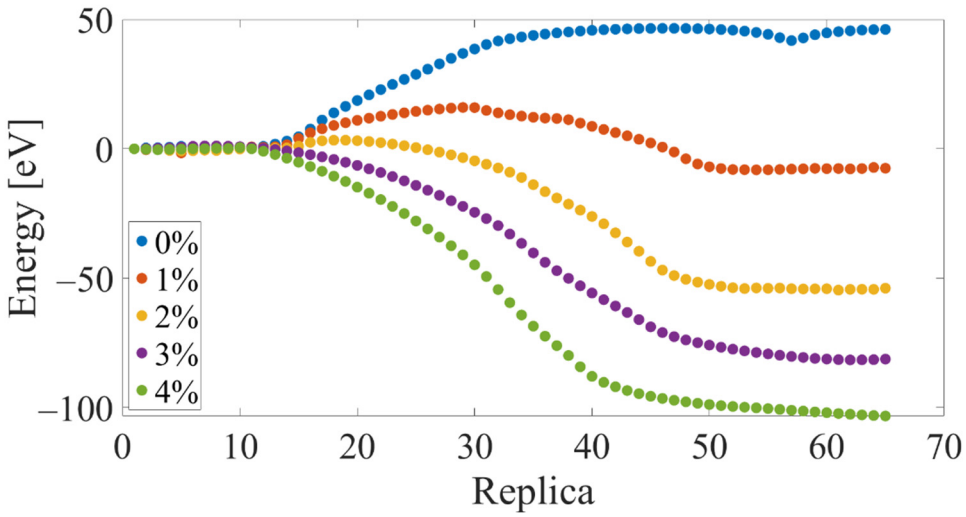


Figure S1. The energy along the minimum energy path between a pristine nanowire and a final state with a dislocation nucleated from the acute angle. Both the initial and final states are strained to the same tensile strain.