Verification of Boundary Conditions in the Experiments: Two ways of fixing the samples were compared. We tested two NWs with similar dimensions, one was fixed to the MEMS testing system using electron beam induced deposition of Pt (diameter=212.6 nm, length=2.55 μm) and the other was fixed by carbon deposition (diameter=223.3 nm, length=2.85 μm). The two NWs were loaded and unloaded three times under the exact same conditions inside a SEM. Figure S1 compares the loading and unloading strain-stress curves of the two samples. In the case of the Pt welded sample, the loading and unloading processes followed the same path and the measured Young’s modulus was 140.4 GPa, in agreement with the modulus computed from stress-SAD strains. In the case of the carbon-welded sample, the unloading curve was different than the loading curve, a clear indication of boundary effects. A low value of Young’s modulus (56.2 GPa) and a large apparent fracture strain (7.73%) was measured indicative of slippage at the
specimen ends. This comparison reveals that the carbon bond is not strong enough to fix large diameter NWs (especially with diameter > 200 nm). These results illustrate some of the challenges in nanoscale testing of mechanical properties and the advantages of in-situ TEM testing.

Figure S1 Stress-strain plots showing the effect of fixing the two ends of the NW via carbon or platinum deposition

**Convergence studies of Wolf’s method of summation:** Bulk ZnO crystal was modeled with periodic boundary conditions in all three dimensions. The energy of the relaxed crystal at 0K was computed with the implemented Wolf’s method of summation, using different values of quasi cut-off radius \(R_c\) and the damping coefficient \(\alpha\). These values were compared with the energy predicted by Ewald method’s of summation, to choose appropriate values for \(R_c\) and \(\alpha\) (as shown in Figure S2). \(R_c=7\text{Å}\) and \(\alpha=0.4\) were used for the simulations presented in this work.
Figure S2 Normalized energy plotted for different parameters of Wolf summation and compared with energy predicted via Ewald summation.