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Stability and Rupture of Ultrathin Ionic Wires

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Abstract

Using a combination of in situ high-resolution transmission electron microscopy (Fig. 1) and density functional theory (Fig. 2), we report the formation and rupture of ZrO2 atomic ionic wires. Near rupture, under tensile stress, the system favors the spontaneous formation of oxygen vacancies, a critical step in the formation of the monatomic bridge. In this length scale, vacancies provide ductile-like behavior, an unexpected mechanical behavior for ionic systems. Our results add an ionic compound to the very selective list of materials that can form monatomic wires and they contribute to the fundamental understanding of the mechanical properties of ceramic materials at the nanoscale.

Figures

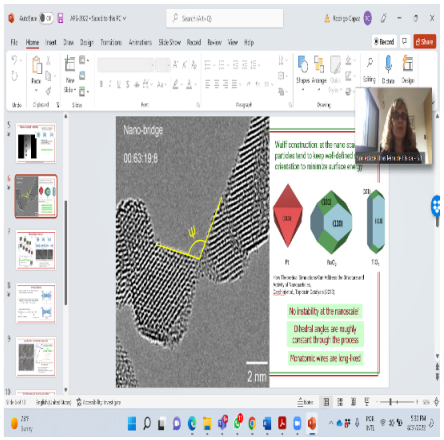

Figure 1: HRTEM image showing a snapshot of the rupture process of ZrO_2 nanoparticles.

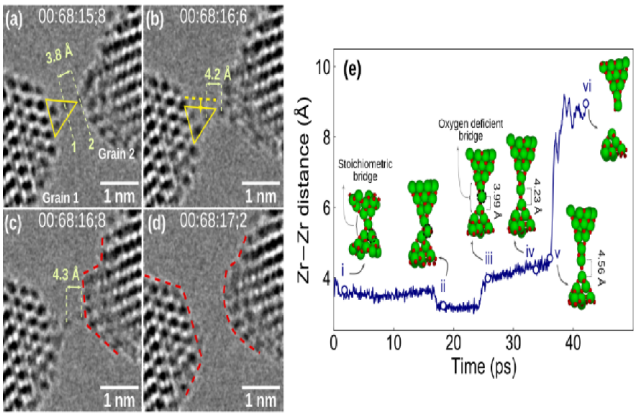

Figure 2: Ab-initio molecular dynamics simulations of the formation and rupture of a ZrO_2 wire.