Deformation and failure of curved nanocrystalline shells

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We study the mechanical response of curved crystalline shells subject to load. These structures, mainly conceived for encapsulation purposes at small scales, show peculiar behavior due to their topological properties, i.e., the minimum energy configuration of any curved crystalline surface contains geometrically necessary topological defects in agreement with its Euler characteristic. The microstructure evolution is therefore influenced by the dynamics of those topological defects on the curved interface and exhibits a rather rich and non-trivial phenomenology. The quasi-static deformation of these structures is characterized by intermittent dynamics with collective particle reorganizations mediated by the proliferation of dislocation pairs and the dynamic delocalization of disclinations in the form of grain boundary scars. At large deformations, depending on bending rigidity, sample size, and geometry, one may observe buckling instabilities and structural failure phenomena such as the cavitation of the crystal shells.

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