Dynamics of topological defects in the mechanical deformation of curved nanocrystalline shells

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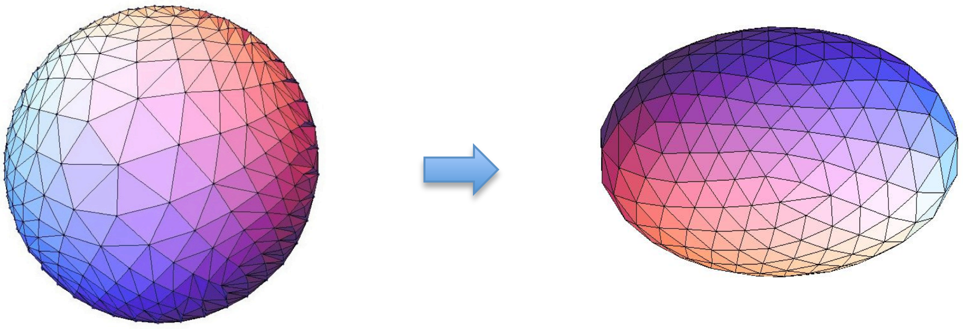
Crystals must deform to fit on curved surfaces. The energy cost associated to such deformations consists of both stretching and bending contributions. According to Euler's theorem and the Euler characteristic of the surface, the minimum energy configuration contains geometrically necessary topological defects, all of which share an elementary building block: the disclination. The elastic cost of a disclination in a crystalline membrane is very high, but buckling and/or the proliferation of boundary scars can reduce it considerably. We briefly discuss the structural transitions and the microstructure dynamics undergoing the continuous mechanical deformation of curved nanocrystalline shells as a function of effective bending rigidity, sample size, and geometry. The quasi-static deformation of these structures is characterized by intermittent dynamics with collective particle reorganizations mediated by the proliferation and dynamic delocalization of defects. At large deformations we eventually observe structural failure phenomena such as the melting or the cavitation of the crystal shells.



Squeezing a spherical nanocrystal: The process involves the nucleation and delocalization of several topological defects. Vacancies and cavities eventually develop at the tips of the spheroid.