The influence of strain-induced ferroelectricity on the fracture of oxide perovskites

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The cleaving of bulk crystals using mechanical force is a common procedure to obtain well-defined surfaces under UHV conditions. While this method avoids chemical changes in the surface composition due to etching and annealing procedures, the strain necessary for cleavage can induce ferroelectric phase transitions during the fracture process whose influence is still visible on the as-cleaved surface, as shown, for example, by Sokolović et al. [1] for mechanically cleaved SrTiO3. Here, we present density-functional theory calculations to discuss the influence of increasing strain on the magnitude of possible ferroelectric distortions and the development of a spontaneous polarization for three prototype perovskite oxides: cubic SrTiO3, ferroelectric BaTiO3, and polar KTaO3. First, we estimate the critical strain for mechanical cleavage in fracture Mode 1 and Mode 2. Subsequently, we calculate the polarization of the material at the point of fracture and discuss the implication on surface charges and the formation of surface defects.

[1] I. Sokolović, M. Schmid, U. Diebold, M. Setvín, *Phys. Rev. Mater.* **2019**, *3*, 034407