Plastic Deformation and Twinning Mechanisms in Magnesian Calcites: a Non-Equilibrium Computer Simulation Study

Sanha Lee, Gøran Svaland [C, S] and Fernando Bresme
Department of Chemistry, Imperial College London, London, United Kingdom, United Kingdom
g.svaland15@imperial.ac.uk

Deformation twinning is a mechanical response to applied stress, where the crystal molecules reorder along planes instead of fracturing. Biological exoskeletons of calcite and magnesium containing calcites can dissipate applied stresses very effectively through such mechanisms [1,2]. While uniform incorporation of magnesium into the crystal lattice of calcite increases its stiffness[2] and hence hardness and wearability, it makes the crystal more brittle and less able to deform by twinning [3]. In order to understand the impact of the arrangement and concentration of incorporated Mg^{2+} ions on the stress relaxation mode, we performed atomistic simulations of uniaxial deformation along the c-axis of magnesian calcites. We cover a wide range of compositions (0, 16, 33, 50, 66, 84 and 100) mo l% Mg^{2+}. We show that magnesian calcites below 50 % Mg:Ca ratio deform by twinning along the (1014) plane and at about 2 % less strain than for pure calcite, whereas at higher concentrations, the crystal fractures at about 2 % more strain than for pure calcite. The stress dissipation in the crystal depends both on the Mg^{2+} content and its arrangement in the crystal lattice. Above 33 mol % MgCO3 the Mg^{2+} ions form a percolating network, and the crystals display a plastic behavior before yield or twinning.

References:

[1] L. Li and C. Ortiz (2014), Nat. Mat. 13(5), 501-7, “Pervasive nanoscale deformation twinning as a catalyst for efficient energy dissipation in a bioceramic armour”
[2] A. Côté, R. Darkins, D. M. Duffy (2015), PCCP, 17(31) 20178-20184, “Deformation twinning and the role of amino acids and magnesium in calcite hardness from molecular simulation”
[3] Zhu et al. (2013), J. Mech. Behav. Biomed. Mater. 20 296-304, “Ab initio study of single-crystalline and polycrystalline elastic properties of Mg-substituted calcite crystals”