Predicted surface structure and crystal growth mechanism of a natural zeolite

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Controlling crystal morphology is an important part of manufacturing materials in established and emerging technologies. The ability to predict the structure and shape of nanoporous materials could have considerable impact upon the crystal engineering of zeolite membranes. A combination of results from classical and first-principles atomistic calculations predicts the surface structure of a natural zeolite (edingtonite). Analysis of the structure and stability of each crystal face indicates that the relative growth rate of faces is found to correlate strongly with the number of broken bonds per unit area formed upon cleaving a given crystal face, whilst the broken bond density is found to be inversely proportional to the surface energy. It can be deduced therefore that terrace nucleation sites on the surface control the rate of growth (rather than steps or kinks) of this material. Inspection of the surface structures, component species and solution species suggests at least two different possible monomer/oligomer mediated self-assembly mechanisms occur during crystal growth. Other natural zeolites from distinct topological families also appear to express a correlation between crystal growth rate and terminating bond density and hence this relation may be exploitable in the characterisation of crystal samples and tailoring of crystal morphology for molecular sieving and catalytic applications.