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Crystal shapes, triglyphs, and twins in minerals: The case of pyrite

Corinne Arrouvel[1,*]

[1]DFQM/CCTS, Universidade Federal de São Carlos, Campus Sorocaba, Sorocaba SP, Brazil

Abstract

The euhedral shapes of pyrite FeS_2 are usually exposing three main surfaces: striated (001), smooth (111), and striated (210), leading to the cubical, octahedral, and pyritohedral morphology, respectively. The macroscopic striations, sometimes called triglyphs on cubic crystals, are parallel on specific surfaces and aligned to the <100> directions. Other types of striated and unstriated (*hkl*) surfaces can be observed on pyrite crystals from Peru, a country offering a rich diversity of pyrite shapes. A rare specimen from Elba Island (Italy) is a pyritohedron with uncommon directions of striations (so-called "negative" striations, first described in Japanese minerals). The Wulff kinetic growth and the periodic bond chain (PBC) theories were not relevant enough to explain crystal shapes, the texture of the surfaces, and twinning. To bring some new insights on crystal growth, twinning, and anisotropy, pyrite samples are analyzed using XRD, SEM, and EDS techniques coupled with atomistic simulations. A first analysis points out that sulfur terminations play a key role in the growth of striations in distinguishing the six <001> directions. The negative striated pyritohedral pyrite would be, in fact, a special case that has stabilized the {120} surfaces, which are structurally different from the {210} facets. The {120} surface has a slightly higher surface energy than the {210} surface (surface energies of 1.68 and 1.65 J/m^2, respectively, calculated with force field methods). {120} pyritohedra from Elba, Italy, are growing next to micaceous iron oxides (a type of hematite), which are also peculiar specimens with magnetic properties. Another specificity is that some rare earth elements have been identified in the pyrite sample from Elba, which leads to a hypothesis that geothermal conditions favor "negative" striations (e.g., discernible in Akita prefecture-Japan, Boyacá-Colombia, and Cassandra-Greece). The striation directions become useful to distinguish (*hkl*) surfaces and to identify twinning as they follow the same patterns on each interpenetrated crystal. The most common twinning is the "iron cross," a penetration twin of two crystals defined by a rotation of 90° along an [001] axis with a coincidence in the iron sub-lattice (e.g., twinning by merohedry) and with a twin center. The sulfur network also plays a fundamental role in stabilizing the (001) interface and in keeping the chemical bulk properties at the boundary, as confirmed by additional ab initio simulations. The grain boundary is a 2D defect in which the (001) twinning is relatively stable as it is common. The calculated formation energy of the rotation twinning is 0.8 J/m^2. The rotation twinning is associated with an apparent reflection on (110) planes. The formation energy of the (110) mirror grain boundary is 1.7 J/m^2, and the interface at the atomic scale is relatively uniform in agreement with experimental observations.

Keywords: FeS_2, crystal growth, force field, anisotropy, Fe_2O_3, Elba, geothermal