Pyrite: A Bond-valence approach to describe crystal growth and dissolution processes

Mutter, Andreas[1] Klingl, Andreas[2] Etzel, Katja[3]
[1]CAU Kiel [2]Universität Regensburg [3]CAU Kiel

The intent of the research presented is to introduce a methodology, which can easily be referred to, while describing crystal growth processes, as well as mineral surface reactions. The strength of this model is its fundamental concept based on the principles of the bond-valence theory (Brown, 2002). Here we will demonstrate how the Bond-valence deficiency model (Mutter 2007) can be applied to describe the morphology of pyrite crystals as well as the morphology of etch-pits formed during abiotic and biotic leaching experiments.

In the past the bond-valence theory has proven to be a valuable tool and is readily applied in order to refine internal crystal structures, by surveying for example the number and "strengths" of bonds formed between the constituents of a crystal. Diverging bond-valence sums around an atom within the crystal structure are treated as an indication of possible defects in the crystal structure, or even worse indicate an insufficient crystal structure analysis. On the other hand, missing bond-valences or insufficient bond-valence sums are natural to atoms at mineral surfaces, and to a large extend these unsatisfied bonds control the readiness of a crystal surface to participate in chemical reactions. The number and thus the "strength" of these bonds can easily be calculated and is addressed as the bond-valence deficiency of an atom, ion, molecule or crystal surface. Obtained bond-valence deficiencies of different crystal faces of a mineral are comparable, and can be used as indicators to predict the crystal morphology. As an example the BVD-values of different pyrite surfaces (100), (111), (210), (211) and (221) are presented, and their morphological importance will be discussed.

Further, as the bond-valence theory can be applied to crystal surfaces and solvents alike, it can be used to interpret the processes and interactions occurring at crystal surfaces, at the interfaces between a solid and a solution. Internal crystal factors, such as crystal symmetry, lattice density and reticular have been effectively combined and can be addressed as factors taking control of the basic topology of the mineral surface. This topology is named the "surface matrix", a theoretical crystal surface, which is able to interact with external factors, such as ions present in a solution. Both aspects, internal and external, can be factorised via the bond-valence deficiency model and their individual influence on minerals surfaces can be calculated. As an example how both factors interact at mineral surfaces the morphology of etch-pits formed on differently oriented pyrite surfaces will be calculated, and these theoretical results will be compared to experimental observations.

References

Brown, I.D.(2002) The chemical bond in inorganic chemistry. Oxford Science Publications

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