Geophysical Research Abstracts,
Vol. 10, EGU2008-A-08288, 2008
SRef-ID: 1607-7962/gra/EGU2008-A-08288
EGU General Assembly 2008

The Bond-Valence Deficiency model: A new approach to describe mineral surface processes

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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. This model is proposed to be a tool, a method to be applied when approaching mineral surface reactions for the first time. It may to some extend be an alternative to molecular dynamic simulations, in so far, as predictions of crystal morphologies and minerals surface reactions are possible and can be obtained in relative short time periods. The strength of this model is its fundamental concept based on the principles of the bond-valence theory [1].

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. This new concept of the bond-valence theory can be applied to crystal surfaces and solvents alike, and can be used to interpret the processes and interactions occurring at crystal surfaces, the interfaces between a solid and a solution.

The concept of the “Bond-valence deficiency model” (BVD-model) presented, is based on a combination of different aspects of several crystal growth theories. 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.

[1] I.D. Brown: The chemical bond in inorganic chemistry. Oxford Science Publications. 2002.