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Solid solution phases used as models for complex mineral phases in geochemical computer models

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The recent evolution of water-rock interaction models tries to better represent complex mineral phases in order to take into account their ability to change their chemical composition, as a consequence of the interaction with natural aqueous fluids of changing chemical composition. This is true even for mineral phases as “simple” as oxides or carbonates but becomes crucial for more complex phases like silicates and particularly clay minerals, formed as alteration products, during weathering or hydrothermal processes at relatively low temperatures (0 to 300°C).

We have applied the concept of solid solution in order to solve this problem in our geochemical code KINDIS [1] and coupled transport/reaction model KIRMAT [2]. Clay minerals, in particular, are represented by generalized n-end-member solid solutions. These tools are now able to produce mineral phases as solid solutions of n-end-members at equilibrium with the aqueous reaction phase or under kinetic control.

However, if one considers mineral phases produced as microsize particles, our approach led us to reconsider the problem of crystal growth modelling for these particular phases. It appeared that it was no longer possible to simply consider either the thermodynamic approach of the problem or the kinetic control. It seemed necessary to combine both approaches with a more thorough description of nucleation and growth processes. This is now under development in a cooperative action between geochemists and physicists (Noguera et al., this issue).

References

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1.4.14

Relationships between crystal morphology and Ba/Sr distribution coefficients in the (Ba,Sr)SO_4-H_2O solid solution-aqueous solution system

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Frequently, marine barite-celestite solid solution is used as a monitor of the strontium, sulphur isotope compositions and ocean productivity [1]. Although the exact mechanism of formation of barite-celestite crystals from seawater is not completely known, they are traditionally distinguished from hydrothermal barite-celestite crystals using morphological criteria [2]. Therefore, it is of interest to determine the relationships between composition and crystal morphology in the (Ba,Sr)SO_4-H_2O solid solution-aqueous solution (SS-AS) system .

We have used the gel method to grow $Ba_xSr_{1-x}SO_4$ crystals from starting aqueous solutions with a wide range of Ba/Sr ratios. Scanning electron imaging and Micropobe analysis of the crystals have revealed a clear relationship between the Ba/Sr content (and distribution coefficients) of the solid solution and the crystal morphology. In addition, for a given crystal morphology, different faces have different distribution coefficients. In order to obtain information of the growth behaviour at a nanoscale in the (Ba,Sr)SO_4-H_2O SS-AS system, in situ Atomic Force Microscopy experiments have been also conducted.

The results have been interpreted on the basis of crystal growth models and SS-AS theory.

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