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Spin Models of Aluminosilicates

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When two pure mineral phases mix and form a solid solution certain types of atoms begin to compete for the same lattice sites. This competition results in the formation of new combinations of atoms with new interaction energies which have not existed in the pure phases. Spin models are aimed to constrain the energies and probabilities of the most important local combinations of atoms (cluster configurations) while probabilities and energies of larger atomic groups can be approximated as certain products and sums of the probabilities and energies of smaller clusters. Using the cluster variation method or Monte Carlo method one can calculate equilibrium properties of a solid solution as functions of a limited number of interaction constants, temperature and composition. The values of the interaction constants can be constrained either directly by available experimental data or can be derived from results of lattice dynamics or ab initio calculations.

Spin models are able to predict locations of order/disorder transitions and miscibility gaps in solid solutions. Moreover, spin models help to understand interesting microscopic `phenomena which lay behind the macroscopic transitions. For example, by analysing the results of a spin model one can see that at a certain temperature an interplay of entropy and enthalpy factors leads to a sudden destabilisation of domain boundaries (cooperative effect) and that at a certain composition cluster probabilities reach internal constrains which prevent further ordering (frustration effect). Using a spin model one can calculate probabilities of certain local atomic configurations and compare them with normalised intensities of an IR or NMR spectrum and thus determine degrees of short-range and long-range order of the atomic distribution. Spin models can also be used to construct images of atomic distributions. Using these images one can visualise domains and domain boundaries. Also, by performing Fourier transformation of the images one can interpret diffuse scattering intensities. The report will be illustrated with several interesting results on spin modelling of aluminosilicates. Among them we will demonstrate the first calculated *T-x* diagram of the subsolidus phase relations in the albite - anorthite system.