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Thermal expansion of Carbonate-Nosean: a phase-transition kinetics model

T. Gesing[1], M. Murshed[1], L. Robben[1]

[1]*University Bremen, Solid State Chemical Crystallography, Inorganic Chemistry GB02, Bremen, Germany*

The description of a Landau phase-transition considers group-subgroup relations with respect to the initial phase at thermodynamic equilibrium. Accordingly, the Gibbs free energy is modified in terms of an order parameter Q [1]. Data collection on a particular phase at equilibrium is challenging in case of associated kinetic effects. Thus describing a phase-transition using the Landau theory leads quite often to a marked discrepancy between the observed and calculated data close to T_c. Evaluating an accurate order parameter consequently must be a hurdle. In some cases the order parameter is proportional to the unit-cell volume of the phase. Similar effect could be seen while evaluating the lattice volume of a phase using Debye-Einstein-Anharmonicity model [2] where the internal energy of a crystalline lattice volume is considered to be sum of the Einstein harmonic, Debye quasi-harmonic and anharmonic vibrational potentials. The DEA-model gives possibility to compare the experimental thermal expansion coefficient (TEC) with that of the theoretical one. For example, in dehydrated carbonate-nosean [3] the kinetic effect close to the P23-P23 phase-transition could be seen in terms of the decrease of the TEC over several data points around 800 K (Figure). In this case, a pure Landau transition would have sharply dropped the TEC leaving no intermediate values. These deviations in the experimental data could be theoretically modeled by overlapping the TEC's of the low-temperature (TEC_{LT}) and the high-temperature (TEC_{HT}) phase using a sigmoidal term f_s (T) {0 < f_s (T) < 1}: TEC_{total} (T) = f_sT•TEC_{low} (T) + (1- f_s(T))•TEC_{high} (T). The slope of this sigmoidal function corresponds to the deviation of the model used for the volume calculation close to the phase-transition and therefore carries information about the reaction kinetics. The same could be calculated for the dehydration process of the hydrated carbonate-nosean $|Na_8(CO_3)(H_2O)_4|[AlSiO_4]_6$ around 400 K. Figure: Experimental temperature-dependent volume change of hydrated carbonate-nosean and respective DEA-model calculation results. The individual DEA-models as well as TEC changes including kinetic overlaps are given inserted.

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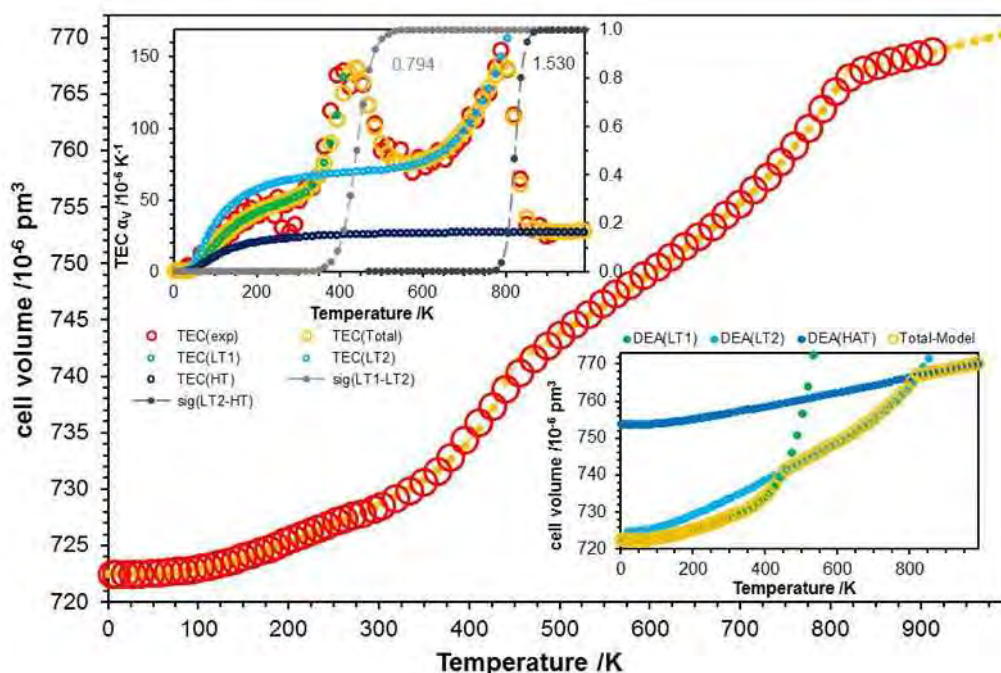
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