21-Crystallography at Non-Ambient Temperatures and/or Pressures: Phase Transitions

The true symmetry of the anions A or template molecules M is of lower grade than cubic symmetry, predominantly in the various SD-compounds under scope. With increasing temperatures the guest/host symmetry mismatch is diminished by dynamics of the guest atoms. They approach spherical character by hopping between equivalent positions with hopping frequencies up to $10^{14}$ Hz close to $T_{dm}$, the temperature of peritectic decomposition of the host structure. $T_w$ is the temperature critical to the guest/host interaction. In the given SOD-compounds the values of $T_w$ vary between 900 and 1500 K for the same type of host composition [X$_2$T$_4$]$_2$O$_{12}$. This given host structure of lattice energy $U_2$ might serve to test the real v. d. WAALS and COU LOMB forces given by the atoms of the guest complexes encapsulated in the 4th-order SOD-cage. There is some evidence for a donor gas character of the guest complexes close to $T_m$, from the high chemical potential provided by the dynamics of the atoms intra-cage rotation, the translational movement being forbidden by the periodic matrix of cages. Upon cooling structural phase transitions occur through cooperation of the guest atoms with the host structure on a certain level of hopping frequencies, thus lowering the symmetry of the host structure[2].

Phase transitions present critical phenomena in the individual type of interactions between the chemical species of the guest- and of the host structure. The rises in the peak shapes by DSC-microcalorimetry.

Some SOD-phases show no structural phase transition, surprisingly, but irregularities in the trace of regular DSC-experiments run with a 5 K/min cooling rate. The shift in the $C_p$-curves, the value of 0.20 J/gK is observed in the hydrosalite type [Na$_2$O[CO(OD)$_2$]$_2$]$_2$[Al$_2$O$_3$]$_2$ at $T_w$ = 150 K, resembles the glass transition of polymers and inorganic glasses. Contrary to the findings in orientational glasses we like to introduce the term dot phase to this group of new materials, which differ by the periodic matrix of cages at in zeolite like materials.

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PS-21.03.21 MECHANISMS OF PHASE TRANSITIONS IN HEXAGONAL MODEL WITH 1q AND 3q INCOMMENSURATE PHASES

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A hexagonal two-dimensional model of particles with displacive degree of freedom and interacting via potential energy with harmonic and anharmonic third and fourth order terms has been studied by molecular-dynamics technique. The phase diagram of the model exhibits normal, k=0 commensurate, one-dimensional (1q) and three-dimensional (3q) incommensurate phases. The 3q phase can be visualized as a sequence of columns, oriented along the hexagonal axis. The columns form a hexagonal incommensurate lattice. At higher temperature, the 3q incommensurate phase is more stable than the 1q phase.

The simulation shows that: (i) The 1q $\rightarrow$ k=0 phase transition is driven by the antiphase, which are topological defects of the stripe and form the third and fourth order term has been studied by the molecular-dynamics technique. The phase diagram of the model exhibits normal, k=0 commensurate, one-dimensional (1q) and three-dimensional (3q) incommensurate phases. The 3q phase can be visualized as a sequence of columns, oriented along the hexagonal axis. The columns form a hexagonal incommensurate lattice. At higher temperature, the 3q incommensurate phase is more stable than the 1q phase.

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