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 SOD-componds under scope. With increasing temperatures the guest/host symmetry misfit is diminished by dynamics of the guest atoms. They approach spherical character by hopping between equivalent positions with hopping frequencies up to $10^3$ Hz close to $T_m$, the temperature of peritectic decomposition of the host structure. $T_m$ is the temperature critical to the guest/host interaction. In the given SOD-componds the values of $T_m$ vary between 900 and 1500K for the same type of host composition $[T_{49}T_TO_{12}]$. Thus a given host structure of lattice energy $U_L$, might serve to test the real v.d.WAALS and CUDLomb forces given by the motion of the guest complexes encapsulated in the $4^{th}$ SOD-cage. There is some evidence for a dot gas charcter 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 $2\times2$ matrix of cages. Upon cooling structural phase transitions occur through cooperition 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 results in the peak shapes by DSC-microcalorimetry show that several SOD-phases show no structural phase transition, surprisingly, but irregularities in the trace of regular DSC-experiments run with a 5K/min cooling rate. The shift in the $c_T$-curves, the value of 0.20 $\Delta c_T$ is observed in the hydrousadate type $[Na_2[ClO_3]_2Al_2Si_2O_7]$ at $T_m$ = 150K, resemble the glass transition of polymers and inorganic glasses. Contrary to the findings in orientational glasses we like to introduce the term dot glass to this group of new materials, which differ by the periodic $2\times2$ matrix of cages at in zeolite like materials.


The excellent magnetic properties of the LaCo$_{13}$ intermetallic compound raised the interest of many researchers. For exploring new rare-earth 3d transition-metal permanent magnets, it is important to investigate intermetallic compounds related to the NaZn$_{13}$ type structure. As is well known, those materials which have cubic structure are impossible to use as permanent magnets because of their high symmetry. From the point of view of crystal structure, we attempt to lower the symmetry of cubic NaZn$_{13}$ by proper heat treatment or elemental substitution, in order to improve magnetic anisotropy.

After annealing at 773K for about two months, structural transitions from cubic to orthorhombic have been observed for LaFe$_3$Al$_3$ (x=6.7). The results of X-ray diffraction and magnetic measurements show that under the given heat treatment procedure, only those cubic NaZn$_{13}$ phase samples with micromagnetic character change their structures. Selected-area electron diffraction patterns confirm that, after annealing at 773K, LaFe$_3$Al$_3$ have a body centered orthorhombic structure with a structural modulation along the a-axis. For LaFe$_3$Al$_3$, the modulated period is 0.068a* (a* = 8.21Å). The structural transitions result in the change of magnetic properties from magnetism to ferromagnetism.

PS-21.03.23 INVESTIGATION OF THE FERROELECTRIC TRANSITION IN POTASSIUM IODATE. By J.G. Zhang, Institute of Crystal Materials, Shandong University, Jinan, China.

Potassium iodate crystals are ferroelectric and belong to the triclinic system with space group P1. They possess thermoelectric properties in the range from -15°C to +300°C. Inversion spontaneous polarization along the pseudo three-fold axis is observed. Four phases exist in this temperature range: the first one exists above 212°C, the second one between 72 and 212°C, the third one between -15 and 72°C, and the last one below -15°C.

Monodomain and multidomain crystals with good optical characteristics were selected. Observations were performed on 2-mm thick (001) ground and polished plates. An investigation of the ferroelectric transition was carried out using an OPTON polarizing microscope, a Leitz heating stage, a long-focus objective lens and a thermocouple temperature measurement device with automatic compensation.

In the hexagonal structure of KIO$_3$, potassium ions are at the vertices, oxygen ions at face centers and iodine ions at body centers. The crystals are paraelectric in phase I. In phase II, iodine ions move along the body diagonal, and spontaneous polarization takes place with formation of 120° domains. In phase III, iodine atoms move perpendicularly to the oxygen ions in one of its planes, and crystals become triclinic. Below 212°C, potassium iodate crystals are mostly 120° and 60° multi-domain crystals.

PS-21.03.24 CHANGE OF LATTICE PARAMETERS AS EVIDENCE OF AUSTENITE THERMAL INSTABILITY IN MANGANESE STEELS. By V.E. Danielsen, A.V. Nedolya* and V.M. Nazarov, Metal Physics Institute and Department of Physics, Zaporizhze State University, Ukraine.


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