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

Krzysztof Partnitski & Gérald Chapuis*

Institut de Cristallographie, Université de Lausanne, BPS, 1015 Lausanne, Switzerland

(On leave from the Institute of Nuclear Physics, Cracow, Poland)

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 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 discommensuration 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 antisites, which are topological defects of the stripe. (ii) In the 3q \( \rightarrow k=0 \) transition, the columns are suppressed. The first eliminations occur at random, the following ones rather close to already annihilated columns. (iii) The 1q \( \rightarrow 3q \) phase transition preserves the modulation wavelength, driven by anisotropic antisites nucleated equidistantly on the discommensuration planes of the 1q phase. The appearing 3q phase may contain deperiodization (dislocation) loops at the sites of a hexagonal discommensuration lattice. (iv) In the 3q \( \rightarrow 1q \) phase transition with constant modulation wavelength, the columns of phase 3q merge into each other to form a stripe of discommensuration plane. (v) The mechanism of the 3q \( \rightarrow 3q \) phase transition associated with a change of the modulation wavelength, exhibits three types of deperiodization loops.

PS-21.03.22 STRUCTURAL TRANSITIONS AND MAGNETIC PROPERTIES IN \( LaFe_5Al_4 \) SYSTEM. By W.H. Tien*, J.K. Liang, X.H. Yan, G.H. Rao, and S.S. Xie, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China.

The excellent magnetic properties of the \( LaCo_{13} \) intermetallic compound raised the interest of many researchers. For exploring the new rare-earth 3d transition-metal permanent magnet, 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 be used as permanent magnets because of their high symmetry. From the point of view of crystal, 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 \( LaFe_5Al_4 \) (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 this, after annealing at 773K, \( LaFe_5Al_4 \) have a body centered orthorhombic structure with a structural modulation along the a-axis. For \( LaFe_5Al_4 \), the modulated period is 0.068\( \AA^1 \) (the 8.2\( \AA^1 \)). 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 ISODATE. 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 \( P\bar{1} \). They possess ferroelectric properties in the range from -18°C to +300°C. Irreversible 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.

Monoclinic 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 the center, and iodide 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 or (100) 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. Danilchenko, A.V. Nedyalkov and V.M. Nudakov, Metal Physics Institute and Department of Physics, Zaporozhie State University, Ukraine.