

Raman and structural studies on potassium-ammonium dehydrogenate phosphate system

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Abstract – Mixed crystals of potassium dehydrogenate phosphate (KDP) and ammonium dehydrogenated phosphate (ADP), were grown at room temperature $25 \pm 2^\circ\text{C}$ by evaporation technique from the supersaturated aqueous solution of the mixed of KDP and ADP for ammonium concentration: $x=0.1, 0.2, 0.3, 0.4$. The competitive growth between NH_4^+ and K^+ ions is important factor which leads to the reductions of the growth rate along the c -axis. The Raman spectra mixed crystals showed that of thermal dehydration as in KDP-system associate with H_2O liberates from KADP_x , and the content of ammonium decreases the transition temperature

In this work, single crystals of $\text{K}_{1-x}(\text{NH}_4)_x\text{H}_2\text{PO}_4$ (KADP_x), were grown by slow evaporation technique. Crystals of different compositions were grown by changing the percentage weight of the KDP and ADP in the solution of the mixed at ambient temperature and pressure. The ammonium concentrations in the mixed solutions were; 0.1, 0.2, 0.3, and 0.4. The starting precursors used in all experiments were analytical grade

The room-temperature X-ray diffraction seems to indicate that the mixed crystal has the same structure as pure KDP (or ADP) but with a lattice constant halfway between that of KDP and ADP (Fig.1). Our observation can be in agreement with the report in [1].

The spontaneous Raman spectra recorded in the $x(\text{zz})y$ -polarizations the scheme for KADP_x are shown in Fig. 2 and Fig. 3 under ambient pressure and function temperature. The observed line shapes reveal appearance of the ν_4 ν_1 modes in the spectra indicates that the local sites symmetry of the PO_4 tetrahedron is C_2 , which is the average symmetry of the paraelectric phase (distorted). In these figures, the results indicated that of the extent of thermal dehydration as in the KDP-type crystals. During the course of dehydration H_2O liberates from the KADP_x structure with the formation of various polymeric intermediates $\text{P}_2\text{O}_7^{4-}$ [2]. On the other hand, the high temperature region coexisting mixed phases appear over large temperature range and with the content of ammonia decreases the transition temperature.

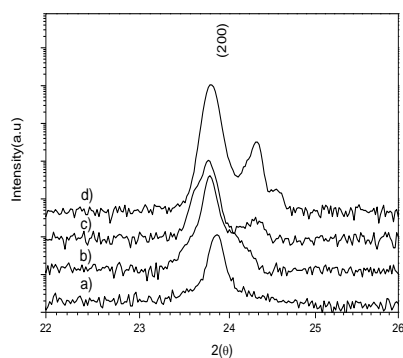


Figure 1: Evolution of X-ray diffraction patterns of KADP_x crystal at room temperature, a) $x=0.1$, b) $x=0.2$ c) $x=0.3$, d) $x=0.4$

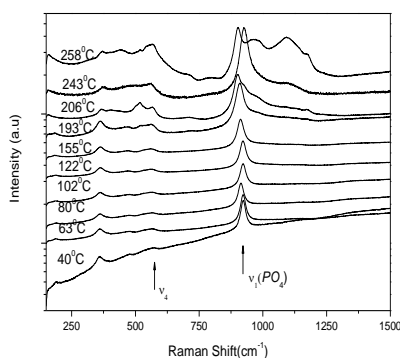


Figure 2: Raman spectra of KADP_x system for $x=0.1$, taken at various temperatures. The internal ν_1 mode of PO_4 vibrations of tetragonal

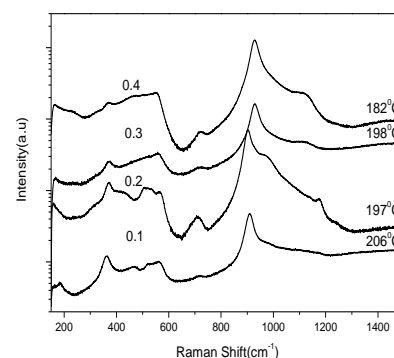


Figure 3: Raman spectra of KADP_x system for $x=0.1, 0.2, 0.3$, and 0.4 taken at various temperatures

References

- [1] Dongli Xu, Dongfeng Xue, J. Cryst. Growth, 310 (2008)1385
[2] Lee, K.-S., J. Phys. Chem. Solids, 57(1966)333