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$K_3Fe_5F_{15}$: FERROELECTRIC AND FERROELASTIC BEHAVIOR

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Ferroelectric oxides with structures related to that of tetragonal potassium tungsten bronze, such as $Ba_2NaNb_5O_{15}$, $K_3Li_2Nb_5O_{15}$ and $PbNb_2O_6$, have been well known for over twenty years. Partial substitution of oxygen by fluorine has recently led to the preparation of new oxyfluorides for which the Curie temperature is strongly depressed even by minor substitution, e.g. in $Ba_{2-x}Na_{1+x}Nb_5O_{15-x}F_x$, T_c = 835K for x = 0 and 100K for x = 1. Ferroelectricity in $K_3Fe_5F_{15}$, an orthorhombic material with distorted tetragonal tungsten bronze-type structure, had been predicted on the basis of its previously reported atomic arrangement. The predicted T_c was 535K whereas the experimental T_c = 490 ± 10K as given by the dielectric permittivity maximum and the λ-type heat capacity anomaly. $K_3Fe_5F_{15}$ is both ferroelectric and ferroelastic, with full coupling between these properties below T_c. The ferroelastic domains disappear sharply on heating above T_c as the symmetry changes from mm2 to 4/mmm. The phase transition was also predicted to be accompanied by a change from order to disorder among the Fe^{2+}, Fe^{3+} ions on heating above T_c, and the prediction is confirmed by the thermal dependence of the Mössbauer effect in which lines due to Fe^{2+} broaden as an anomaly appears in the hyperfine structure at T_c.