CRYSTALLOGRAPHIC STUDY AND PHASE TRANSITIONS OF Sr(Ti, Li)(O, F)$_3$ OXIFLUORIDES

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ABO_3 perovskites have various properties and are attractive for electronic devices. Among these materials, $BaTiO_3$ is the best-known example which has been intensively studied worldwide while the studies on $SrTiO_3$ are limited. The solid solution $Ba_{1-x}Sr_xTiO_3$ is of particular interest for the development of small size integrated circuit memories. In a previous work, we have investigated the system $SrTiO_3 - SrF_2 - LiF$ and several oxifluorides with general formula $Sr(Ti_{1-x}Li_x)O_{3-3x}F_{3x}$ were obtained. The purpose of this study is to determine the lattice parameters and the phase transitions of these new compounds.

Various mixtures [(1-x) $SrTiO_3$ + x SrF_2 + x LiF] are prepared and then heated at 1223 K in air atmosphere for 2 hours. The purity and the symmetry of the obtained samples are checked by X-ray diffraction. A new solid solution occurs in the $0 \leq x \leq 0.40$ starting composition range. The powder patterns of pure $SrTiO_3$ and $Sr(Ti_{1-x}Li_x)O_{3-3x}F_{3x}$ are very different one from others. The oxifluoride phases are isostructural and crystallize with a complex perovskite structure isomorphous to $NaNbO_3$ whereas the strontium titanate is cubic. The unit cell parameters are determined at room temperature and refined using least squares refinement.

Taking into account the lattice symmetry, it is not excluded that the $Sr(Ti_{1-x}Li_x)O_{3-3x}F_{3x}$ compounds undergo several phase transitions like $NaNbO_3$. To make clear this hypothesis, Differential Scanning Calorimetry (DSC) analyses are performed on powder samples from 300 to 873 K. In any case, three phenomena, which could be attributed to structural changes, are observed on the DSC curves. These phase transitions appear respectively at $530\ K \leq T_1 \leq 560\ K$, $640\ K \leq T_2 \leq 680\ K$ and $710\ K \leq T_3 \leq 850\ K$. These new oxifluorides are more interesting than conventional dielectrics for many practical applications.

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