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## Structural evolution and dopant occupancy preference of yttrium-doped potassium sodium niobate thin films (Article)

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### Abstract


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Sodium potassium niobate (KNN) is the most promising candidate for lead-free piezoelectric material, owing to its high Curie temperature and piezoelectric coefficients among the non-lead piezoelectric. Numerous studies have been carried out to enhance piezoelectric properties of KNN through composition design. This research studied the effects of yttrium concentrations and lattice site occupancy preference in KNN films. For this research, the yttrium-doped KNN thin films (mol% = 0, 0.1, 0.3, 0.5, 0.7 and 0.9) were fabricated using the sol-gel spin coating technique and had revealed the orthorhombic perovskite structures. Based on the replacement of  $Y^{3+}$  ions for  $K^+ / Na^+$  ions, it was found that the films doped with 0.1 to 0.5 mol% of yttrium had less lattice strain, while films with more than 0.5 mol% of  $Y^{3+}$  ions had increased strain due to the tendency of  $Y^{3+}$  to occupy the B-site in the perovskite lattice. Furthermore, by analysing the vibrational attributes of octahedron bonding, the dopant occupancy at A-site and B-site lattices could be identified. O-Nb-O bonding was asymmetric and became distorted due to the B-site occupancy of yttrium dopants at high dopant concentrations of >0.5 mol%. Extra conduction electrons had resulted in better resistivity of  $2.153 \times 10^6 \Omega$  at 0.5 mol%, while higher resistivity was recorded for films prepared with higher concentration of more than 0.5 mol%. The introduction of  $Y^{3+}$  improved the grain distribution of KNN structure. Further investigations indicated that yttrium enhances the surface smoothness of the films. However, at high concentrations (0.9 mol%), the yttrium increases the roughness of the surface. Within the studied range of  $Y^{3+}$  the film with 0.5 mol%  $Y^{3+}$  represented a relatively desirable improvement in dielectric loss,  $\tan \delta$  and quality factor,  $Q_m$ .

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### SciVal Topic Prominence

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Dielectric losses Doping (additives) Ions Niobium compounds Perovskite Perovskite solar cells Piezoelectricity Single crystals Sol-gels Yttrium Yttrium alloys

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