

Defect dipoles-induced domain reorientation of NdFeO₃-PbTiO₃ thin films

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The lattice parameters of the NF-PT film were calculated on the peak values of (100) and (111) in the XRD pattern, which are both identifiable in the GI-XRD pattern. The values of a and c were calculated through the Bragg's Law:

$2d\sin\theta = n\lambda$, where the $\lambda = 1.5416$ nm.

And

$$d_{hkl} = \frac{1}{\sqrt{\left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2 + \left(\frac{l}{c}\right)^2}}$$

$$d_{111} = \frac{1}{\sqrt{\frac{2}{a^2} + \frac{1}{c^2}}}$$

As the film is tetragonal, $a = b \neq c$. Therefore, $d_{100} = a$ and

The peak of the (100) is located at $2\theta = 22.71^\circ$. So, $a = \lambda/2\sin\theta = 1.5416/(2\sin 11.35^\circ) = 3.9148$ Å.

The peak of the (111) is located at $2\theta = 39.62^\circ$. $\frac{1}{\sqrt{\frac{2}{a^2} + \frac{1}{c^2}}} = 1.5416/(2\sin 19.81^\circ)$ and $a = 3.9148$ Å. The value of c could be determined to be 4.0181 Å.