Real time nanoscale observations of domain wall movement and pinning in $Na_{0.5}Bi_{0.5}TiO_3$

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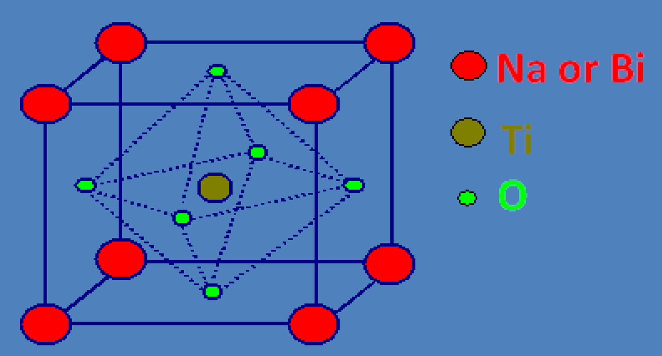
Abstract

Ferroelectric materials are those which possess a spontaneous and reversible electric polarisation. Due to this property, ferroelectric materials are useful for applications in ultrasonic sensors, computer memory devices and can be used as capacitors with a tuneable capacitance. As the behaviour of polarisation domains and their interaction with defects determine the ferroelectric properties, there is a lot of interest in investigating domain wall movement. My project involved using a 200 kV transmission electron microscope (TEM) to study domain behaviour on the nanometre scale.

What is $Na_{0.5}Bi_{0.5}TiO_3$?

$Na_{0.5}Bi_{0.5}TiO_3$ (NBT) is a promising lead-free ferroelectric material with a rhombohedral Perovskite structure at room temperature. As it is also a piezoelectric, NBT has potential applications in transducer sensors, actuators and non-volatile memories.

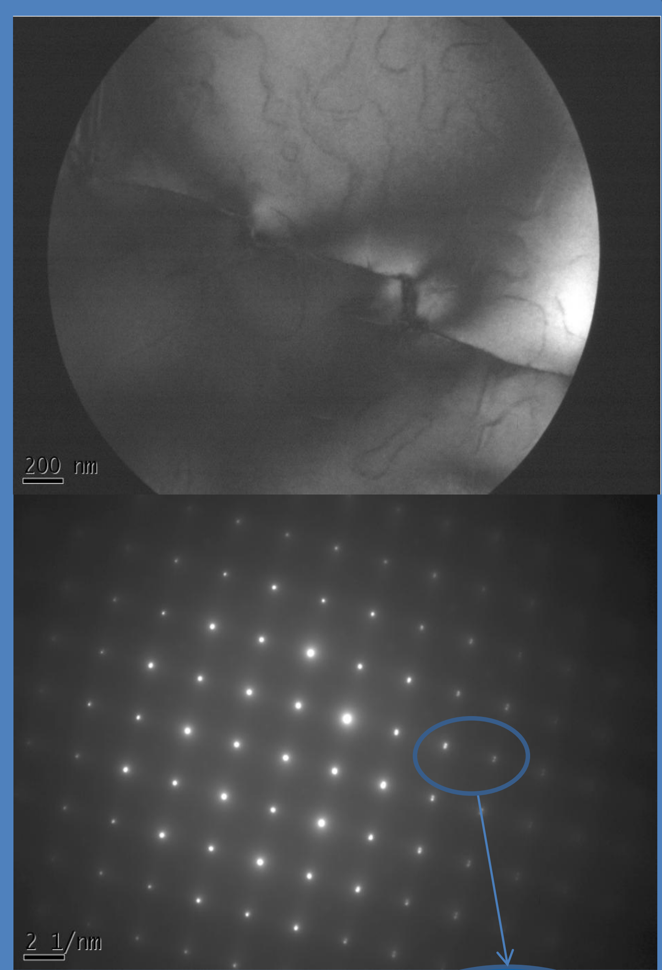


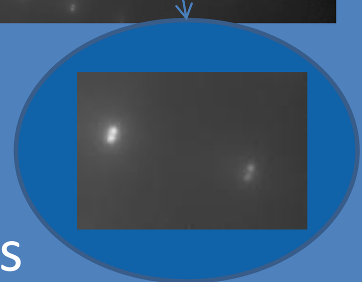
Domain Model

Before using the TEM to obtain any movies, it was necessary to have a model to describe any phenomena that may be seen. By modelling the domain boundary as a mechanical twin boundary between two unit cells of different polarisation, it is possible to find all the allowed types of domain wall. This, in turn, means it is possible to catalogue and understand any phenomena that is encountered. In order to be permissible wall, the unit cells on either side of the wall must satisfy mechanical compatibility conditions in order to minimise the strain energy. This leads to the idea of 'plane matching', which gives a condition to decide whether a wall is permitted or not.

Results

By the end of the project, a substantial amount of video was obtained via a CCD camera, which catalogued a wide range of phenomena. The results that were obtained supported our model. For instance, only two types of twin domain boundaries were observed, which is in agreement with our theory that states that there are only two permissible domain walls. The two images to the right also support the twinning model. The image (*top right*) shows the selected area where the electron diffraction pattern was taken. A (100) domain wall can been seen going diagonally across the image. Underneath the image is the selected area electron diffraction pattern. Notice that there is splitting of the higher order spots. This is because the unit cells are at different orientations on either side of the boundary, which gives rise to slightly different Bragg conditions.

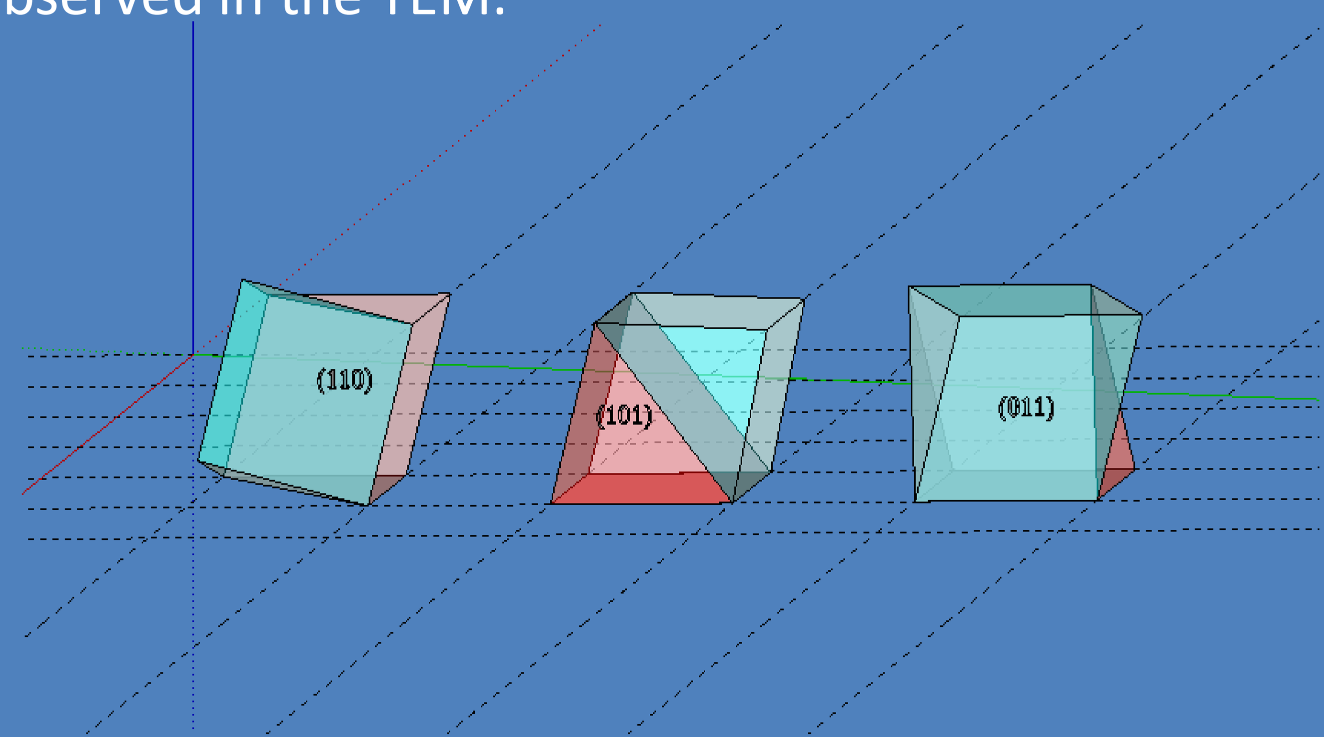




The image (*bottom right*) shows many important features relating to domain structure. The wedge-shaped structures, which alternate between light and dark, are the {110} domain walls. This is evident because, from our model, the {110} walls have both vertical and horizontal extent, which can be seen in the image. A {100} wall is also visible in the image. The top horizontal wedge has been pinned on a defect. As the wedge cannot continue to move forward, it spreads out along a <100> direction, which leads to the formation of a {100} wall.

Permitted Domain Walls

It was found that there are only two different domain walls; those lying on the {100} crystallographic planes, and those lying on the {110} planes. This is consistent with the two different domain wall structures that observed in the TEM.



The diagram shows the model of the 3 orientations of the {110} walls. It shows the original (red) unit cell and its blue twin joined by the domain wall. Notice that the red and blue unit cells match up on the boundary, and hence satisfy the plane matching condition.

URSS Experience

The URSS scheme has allowed me to gain an insight into what academic research is like. The experience I have gained from the project is invaluable in itself, but I have also gained several transferable skills that can be applied to both my degree and future career.

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