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Strain Relaxation by Misfit Dislocations in Nanoscale Epitaxial Ferroelectric $BaTiO_3$ Films Grown on $SrTiO_3$ Substrate

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Integration of electronic oxides into semiconductor devices plays an important role in developing new microelectronic and microelectromechanical technologies. Lattice and thermal expansion mismatch with substrate will introduce significant strains and defects in oxides, and affect its physical properties as well as device performance. Above critical thickness, dislocations will form to accommodate the misfit strain. Understanding strain relaxation mechanism is critical for high quality thin film growth. In this work, we report our studies on the microstructure and defect configurations of $BaTiO_3$ thin films using transmission electron microscopy (TEM).

$BaTiO_3$ is an important ferroelectronic material that has promising applications in various electronic devices. Epitaxial thin films of 8nm, 12nm and 20nm in thickness have been grown on (001) $SrTiO_3$ substrate by reactive molecular beam epitaxy (MBE). There will be ~2.3% lattice mismatch when a stoichiometric tetragonal $BaTiO_3$ (a=0.3994nm, c=0.4038nm) is epitaxially grown on cubic (001) $SrTiO_3$ (a=0.3905nm) substrate with (001)[001]$BaTiO_3$//(001)[001]$SrTiO_3$. Critical thickness was estimated to be 5nm [1]. So misfit dislocation is expected to exist in the films studied in this work.

The major dislocations observed in the $BaTiO_3$ thin films are edge dislocations with Burgers vector $\mathbf{b} = a\langle 100\rangle$. Fig. 1(a) shows a cross section high resolution transmission electron microscopy (HRTEM) image of the 12 nm thick film, in which a full dislocation $\mathbf{b} = a\langle 100\rangle$ is found at the interface. The Burgers vector was determined from the image by drawing a Burgers circuit, as shown in Fig. 1(b). Full dislocations may dissociate into partial dislocations, for example $a[100] = a[10\bar{1}]/2 + a[101]/2$, as shown in Fig.1(c). For the 8 nm thick film, dislocation is mainly located at the interface. For thicker films, dislocations may also occur inside the film, for example the partial dislocation shown in Fig. 1(a-b).

The distribution of dislocations in the film was studied by dark field imaging for both cross section and plan view samples. Fig. 2(a) is a cross section dark field image of the 20 nm thick film under $\mathbf{g}$ = [200] two beam condition. Corresponding selected area electron diffraction pattern (SAED) is shown in Fig. 2(b), in which the separation of (001) diffraction spots from $BaTiO_3$ and $SrTiO_3$ can be identified. Fig. 3(a) is a plan view bright fried image of the 20 nm thick film and corresponding SAED pattern is shown in Fig. 3(b). Dislocation network is seen in Fig. 3(a). Dislocations in the network are edge dislocations with the Burgers vector $\mathbf{b} = a\langle 100\rangle$, determined by dark field imaging [see Fig. 3(b)]. The dislocation line density measured from the network is ~100nm, which is much less than 17 nm calculated for a fully relaxed film. This means that the stress in the epitaxial film is not fully relaxed by the dislocation network. Other type dislocations, such as dislocation loop, half loops, threading dislocations, also exist in the film, which can be seen from Fig. 3(a) and need to be studied in more detail.

In summary, both full and partial misfit dislocations were found in 8nm, 12nm and 20nm thick $BaTiO_3$ films and their structures were studied by HRTEM. Cross section and plan view dark field images were used to study the dislocation distribution and density in the films. The dislocation network can not fully relax the misfit strain. Other type dislocations, such as dislocation loop, threading dislocation, also exist in the film, which may also contribute to the strain relaxation.

Reference:

1. T. Suzuki *et. al.* Philosophical Magazine A79 (1999) 2461.

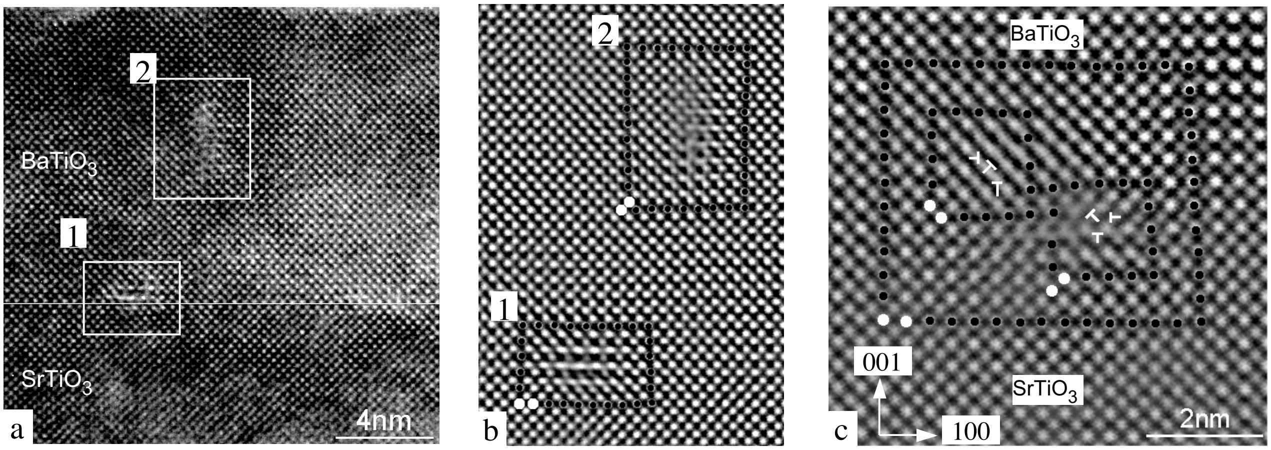

Figure 1 (a) is a HRTEM image of $BaTiO_3$(12nm)/$SrTiO_3$. Burgers vectors are determined to be **b**=a[100] and **b**=a[-10-1]/2 for the defect areas 1 and 2 respectively by drawing Burgers circuits in a Fourier filtered image (b). (c) Dissociation of a full dislocation by the reaction a[100]=a[10-1]/2 +**a**[101]/2.

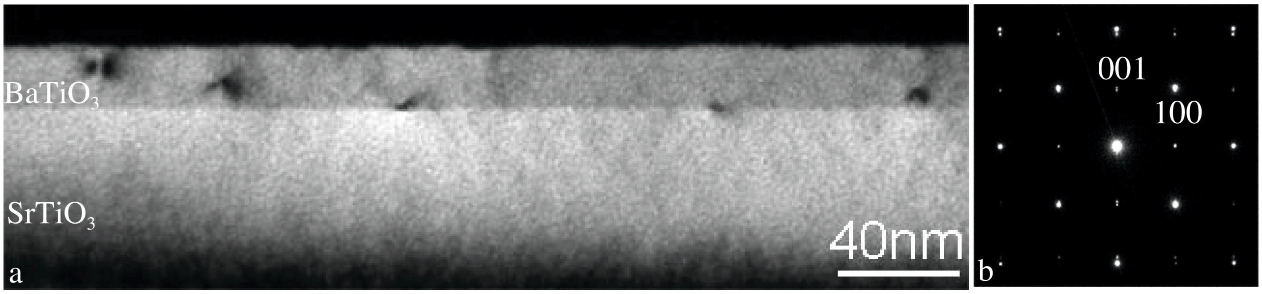

Figure 2 (a) Cross sectional dark field image of $BaTiO_3$(20nm)/$SrTiO_3$ using **g**=[200] two beam condition. (b) Corresponding selected area electron diffraction pattern including both $BaTiO_3$ and $SrTiO_3$.

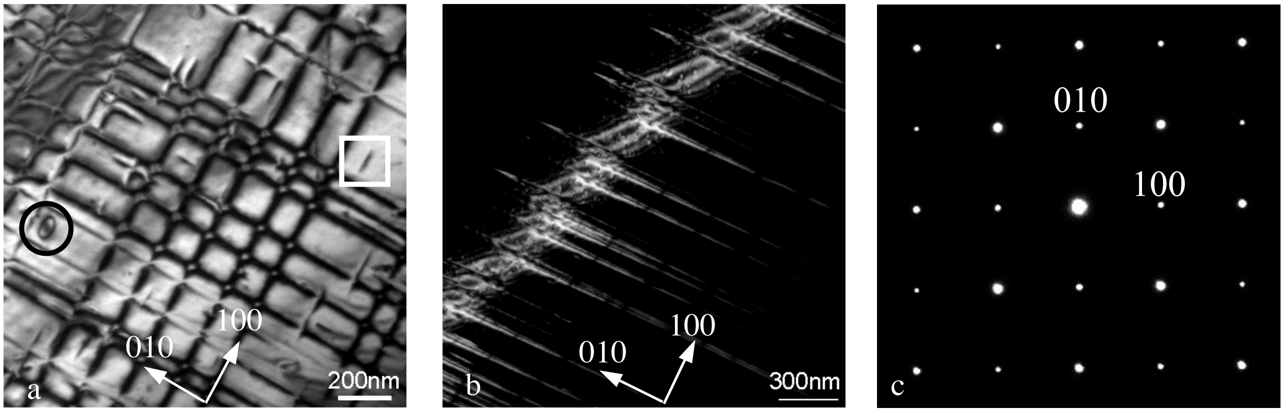

Figure 3 (a) Bright field plan view image of $BaTiO_3$(20nm)/$SrTiO_3$ using **g**=[110] two beam condition, in which dislocation network, loops and half loops can be identified. (b) Dark field image using **g**=[200] two beam condition. (c) Selected area electron diffraction pattern of (a).