Defects in epitaxial $SrRuO_3$ films Grown on $SrTiO_3$ (001) substrate : Misfit dislocations and impurity phase precipitation

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Abstract

Deviation in either chemical composition or lattice parameters of epitaxial oxide films from bulk states can largely influence on the physical properties of heteroepitaxial structures. Off-stoichiometry in film composition can cause secondary phase precipitation, which may be expected or unexpected from equilibrium phase diagram, and lattice misfit between two materials can introduce defects such as misfit dislocations and twin at the interface to accommodate lattice misfit stress. In the present study, we report the transmission electron microscopy (TEM) study on misfit dislocations and the coherent metallic Ru precipitation in epitaxial $SrRuO_3$ films prepared with stoichiometric $SrRuO_3$ target.

The misfit dislocations in $SrRuO_3/SrTiO_3$ heteroepitaxial structure were analyzed by large angle convergent electron diffraction (LACBED) as well as HREM imaging methods [Fig. 1, 2]. Above critical film thickness (~ 8.3 nm), the interface between $SrRuO_3$ and $SrTiO_3$ revealed the square network of misfit dislocations along <100> directions with Burgers vectors of pure edge character a_s<010>. Besides the square network of edge dislocations, pure screw dislocations along [110] directions of $SrTiO_3$ substrate were observed to form along growth steps, due to the orthorhombic nature of $SrRuO_3$.

Metallic Ru precipitates imbedded in primary phase of $SrRuO_3$ have regular "rod-like" shapes and are oriented to the <110> directions of substrate with densities up to $4.2 \times 10^{12}/cm^2$. The excess Ru incorporation of around 2 ~ 7%, which was induced by the difference in sputter yield between Sr and Ru, could cause a eutectoid solidification and resulted in the two-phase composite structure made of single-crystalline $SrRuO_3$ matrix and Ru precipitates. Epitaxial relationship between Ru precipitates and $SrTiO_3$ (STO) revealed to be $(011)_{Ru}//(002)_{STO}$ and $[100]_{Ru}//[110]_{STO}$ [Fig. 3]. This type of in-plane arrangement is

somewhat similar with $\{111\}_{pc}$ ('pc' denotes pseudo-cubic symmetry of $SrRuO_3$) twin occurring at Sr-O planes of $SrRuO_3$ in order to accommodate oxygen deficiency or lattice misfit. The Ru precipitation phenomenon caused 2 nm-deep trenches to be developed on the surface of the 10nm-thick $SrRuO_3$ film along the <110> directions and also would be expected to affect physical properties, such as electrical conductivity, magnetization, and the Curie transition temperature (T_c).

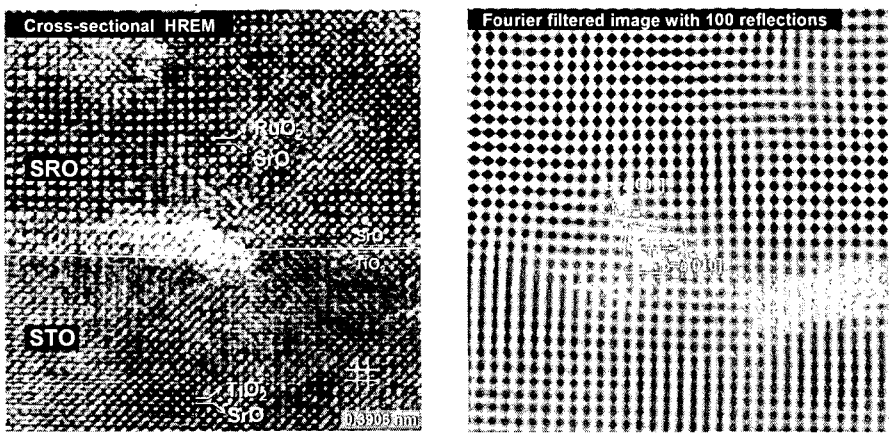
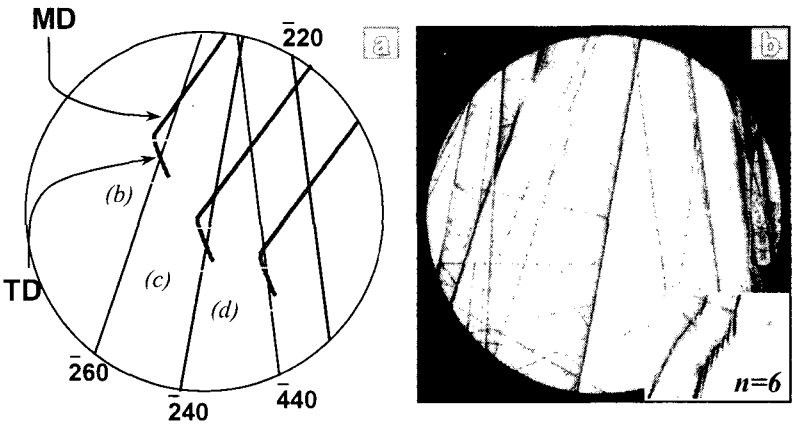


Fig. 1. HREM image of 77 nm-thick $SrRuO_3$ film on $SrTiO_3$ substrate (left) and Fourier filtered image showing the periodicity of <100> lattice planes



(right).

Fig. 2. (a) Schematic illustration of HOLZ lines and dislocation lines used for the **g** · **b** operation. (c) LACBED pattern showing the splitting of 260 reflection line at the crossing position with a threading dislocation connected to a misfit dislocation.

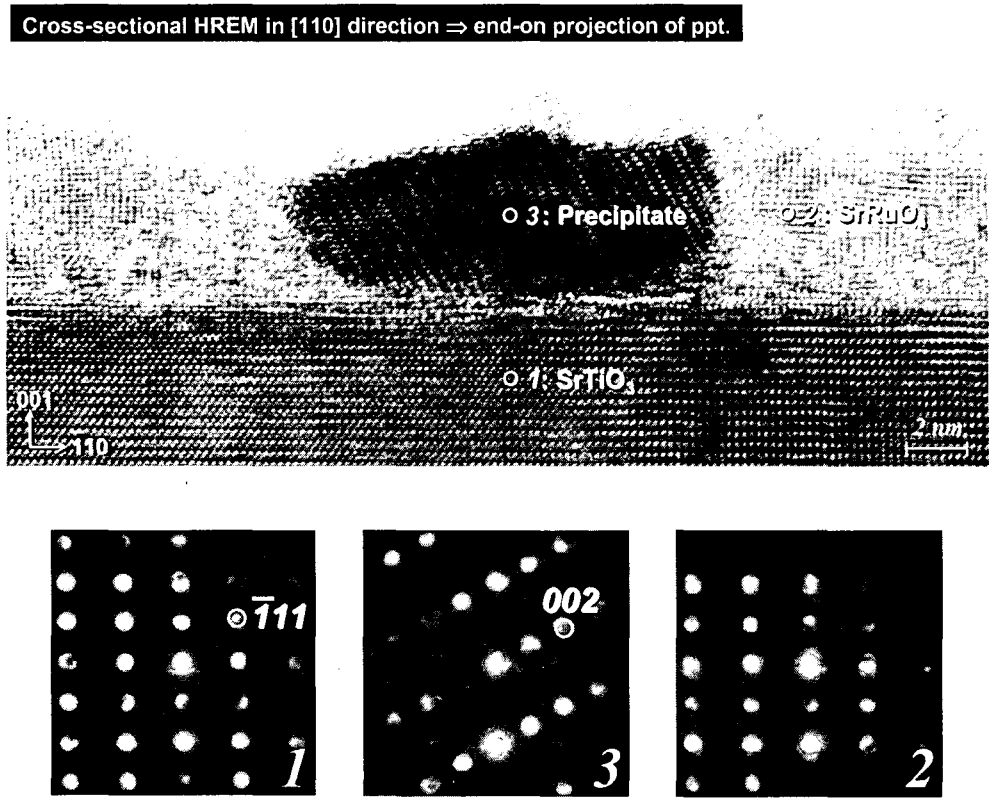


Fig. 3. Cross-sectional HREM micrograph of 10 nm-thick $SrRuO_3$ film on $SrTiO_3$ substrate taken in the [110] direction. Included are the nano-beam diffraction patterns obtained from the $SrTiO_3$ substrate (point 1), the $SrRuO_3$ film (point 2), and the precipitate (point 3).