Misfit strain relaxation mechanism of the SrRuO3 films epitaxially grown on perovskite substrates

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Abstract

Conductive perovskite oxide films, which are chemically and structurally stable in contact with single crystalline substrates, are strongly needed for the successful integration of the memory devices. A metallic conductive oxide, SrRuO3, is a strong candidate material for perovskite heterostructure because of its orthorhombic structure based on a cubic perovskite subcell (*a'* 0.393 nm) and small lattice mismatch with SrTiO3 (*a* 0.3905nm) and LaAlO3 (*a* 0.379 nm) substrates.

However, reliable data on misfit relaxation in epitaxially grown perovskite heterostructure can be hardly found, in contrast to those in the well-developed III-V semiconductors. In the present study, therefore, we have tried to find out the mechanism of misfit strain relaxation of epitaxially grown SrRuO3 films, which depend mainly substrate temperature, film thickness and misfit strain by using high resolution transmission electron microscopy.

Substrate temperature usually affected the surface diffusion length of adatoms on the substrate surface so that it could determine the surface morphology, strain relaxation by misfit dislocation propagation, and consequently the crystal structure. In the temperature region where step flow growth mode is operative, the misfit dislocations propagate by means of both the gliding and climbing of threading dislocations due to 90° geometric confinement of misfit dislocations on the interface. The motion of misfit dislocations are thermally activated process.

When film thickness has exceeded greatly the critical film thickness, active sources for misfit dislocation generation, such as pre-existing dislocations and surface inhomogeneities, are fixed and insufficient especially for misfit relaxation of (001)-oriented $SrTiO_3$ perovskite substrate. The misfit dislocation density was maintained constant independent on film

thickness and thus, films are highly strained. In order to accommodate the excess strain, the meta-stable films experience severe microstructural modifications with the film thickness from dislocation mediated interface into 1) homogeneously strained film with planar faults and further into 2) heterogeneously strained film along the growth direction bounding with undulated surface and mis-oriented interface with respect to substrate.

The effects of substrates exhibiting different lattice mismatches with SrRuO3 film were analyzed as the critical phenomenon for misfit dislocation in terms of forces acting on dislocations. Unlike strain relaxation mechanism of films on SrTiO3 substrate discussed at above paragraph, the films grown on $LaAlO_3$ substrate are readily relaxed above the critical film thickness because the {111} planar defects formation is easily activated due to the large driving force from large misfit strain.

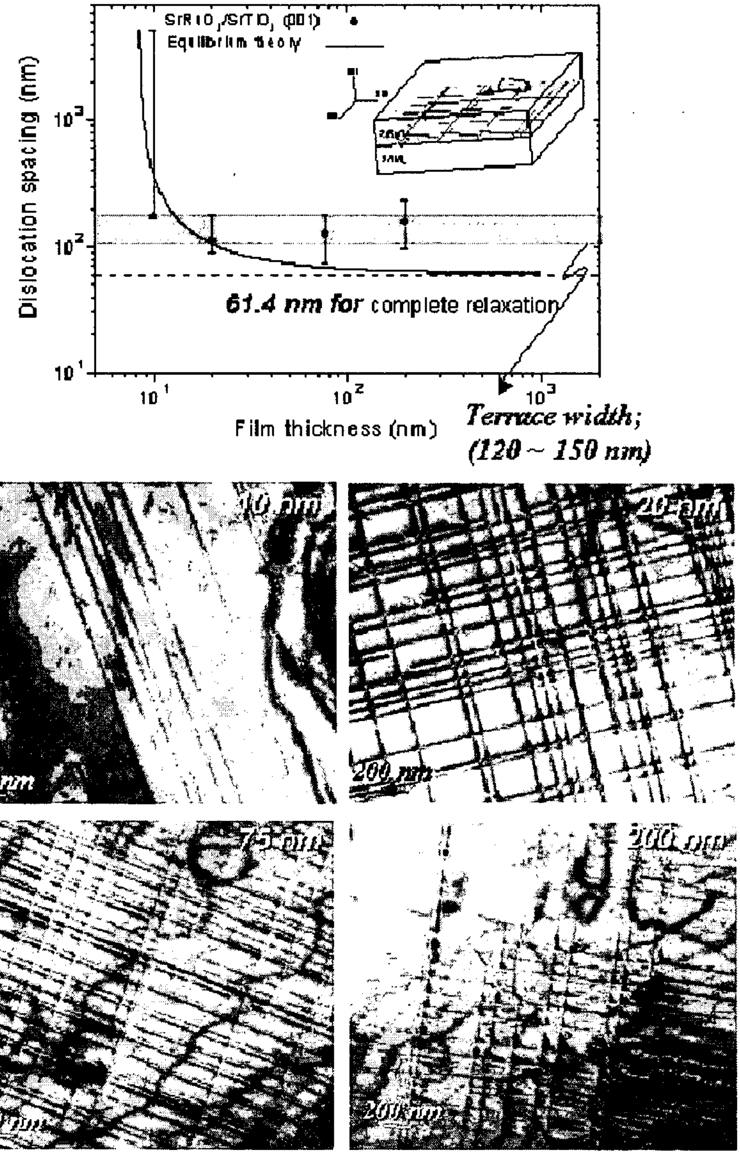

Fig. 1. Metastable equilibrium in misfit strain relaxation of SrRuO3 films on SrTiO3 substrates with respect to increased film thickness.

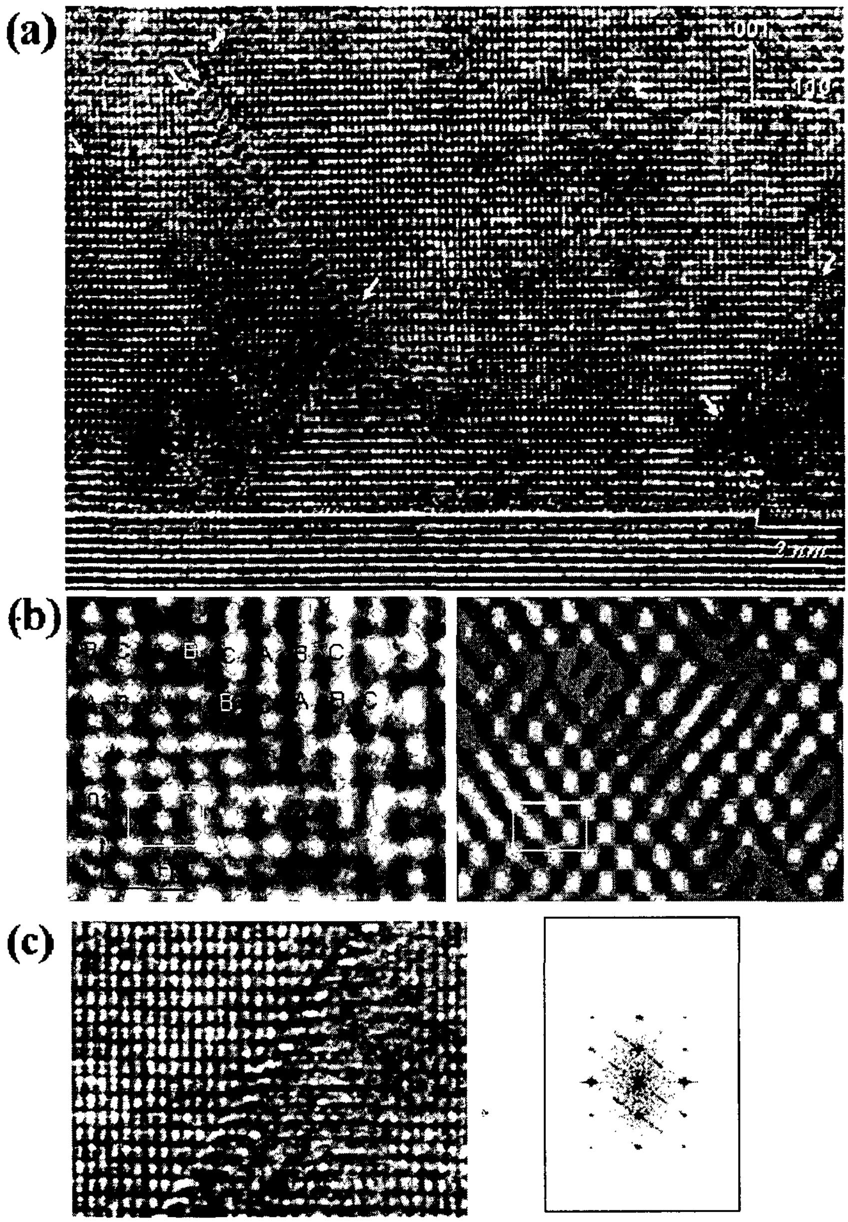

Fig. 2. Planer defects in SrRuO3 thin films grown on LaAlO3 substrates. :
(a) Observation of defects in cross-sectional (110) view,
(b) {111} Frank partial dislocation, and (c) {111} twin