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Microstructures of a Highly Conductive Nb:$SrTiO_3$ Thin Film

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$SrTiO_3$ (STO) has been widely investigated in the past several decades. Conductive doped-STO is of technological interest [1-2]. However, Nb:STO single crystals are expensive and Nb:STO thin films are considered to be a reasonable alternative.

So far work on the doped STO films has been mainly focused on the test of optical and electrical properties. Little work has been done on detailed microstructural characterization, especially on the defect configurations. In this paper, we present a study of the microstructure in the Nb-doped STO thin films, which is expected to shed some light on understanding the high conductivity of the present film.

The computer-controlled laser molecular beam epitaxy (LMBE) system was used to grow the Nb-doped STO thin film. Detailed procedures were given elsewhere [3]. The cross sectional and plan view specimens for TEM observation were prepared by conventional process. A JEOL 2010 high-resolution electron microscope (HREM), with point resolution of 0.194nm and working at 200 KV, was used to carry out contrast analysis and lattice imaging.

In the present film, an approximately periodic array of misfit dislocations is found along the interface, as shown in Fig. 1(Left), in which the positions of misfit dislocations (MDs) are denoted with the vertical arrows. One of them is magnified in Fig. 1(Right) to display the structural details. By drawing a Burgers circuit surrounding the dislocation core, the Burgers vector **b** is determined as *a* [011]. Such a Burgers vector is different from that in the previous work in which it was generally reported that MDs have Burgers vectors of *a* 〈010〉 type [4-5]. It is of great interest to note that the dislocations in the present study are further dissociated into two partial dislocations with 1/2 *a* [011] Burgers vectors, and the two partial dislocations are linked by a stacking fault.

Few threading dislocations were observed in the plan-view specimen, which is significantly different from previous reports related with $SrTiO_3$ [5-6]. Contrast analysis through tilting experiments revealed some characteristics of these MDs. The bright-field images shown in Fig. 2(a), 2(b), and 2(c) were taken under **g** = (110), **g** = (100) and **g** = (010) two-beam conditions, respectively, with an incident beam direction close to [001]. It is seen that when imaged with **g** = (110), two-set of dislocations were in contrast. When imaged with **g** = (100), one of them was out of contrast and another set still kept in contrast with the dislocation line along [010] direction. When imaged with **g** = (010), the above dislocations were out of contrast, however, another set of dislocations were in contrast with the dislocation line along [100] direction. According to the extinction criterion **g• b = 0**, contrast analysis indicates that the highly dense dislocations shown in Figs. 1 are pure edge-type resulting from lattice mismatch between film and substrate.

In summary, by means of transmission electron microscopy we characterized the microstructures of a highly conductive Nb-doped $SrTiO_3$ thin film. One feature at the interface between the film and

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substrate is the array of pure edge misfit dislocations, approximately equally spaced along [100] and [010] directions, respectively, forming the rectangular grid pattern parallel to the interface. It is found that all these misfit dislocations, whose Burgers vectors are $a\langle 011\rangle$, were dissociated into two equal partial dislocations with the Burgers vectors of $a/2\langle 011\rangle$, bounded by a stacking fault. The absence of highly dense threading dislocations is proposed to account for less resistance to the motion of the negatively charged carrier and thus enhances the electron mobility.

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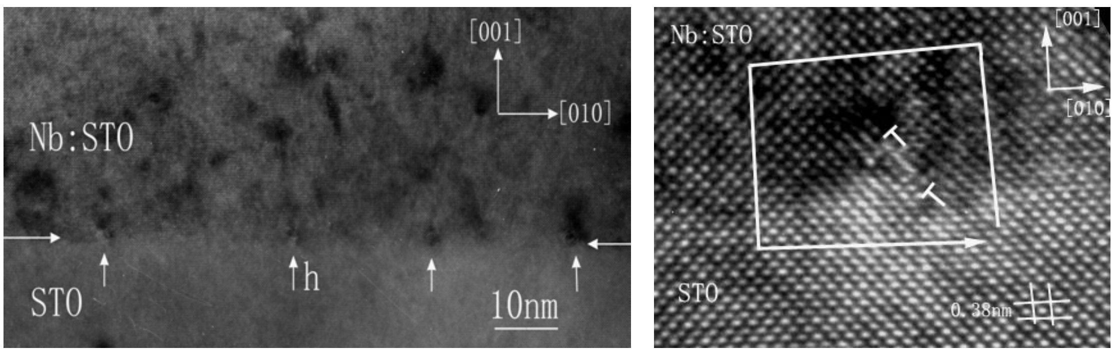

Fig.1. (Left) Cross section lattice image of Nb:STO thin film on (001) STO substrate showing an approximately periodic array of misfit dislocations along the interface. The positions of misfit dislocations are denoted with vertical arrows. (Right) HREM images of a mismatch dislocation (h) in which the Burgers circuit around the dislocation core is outlined.

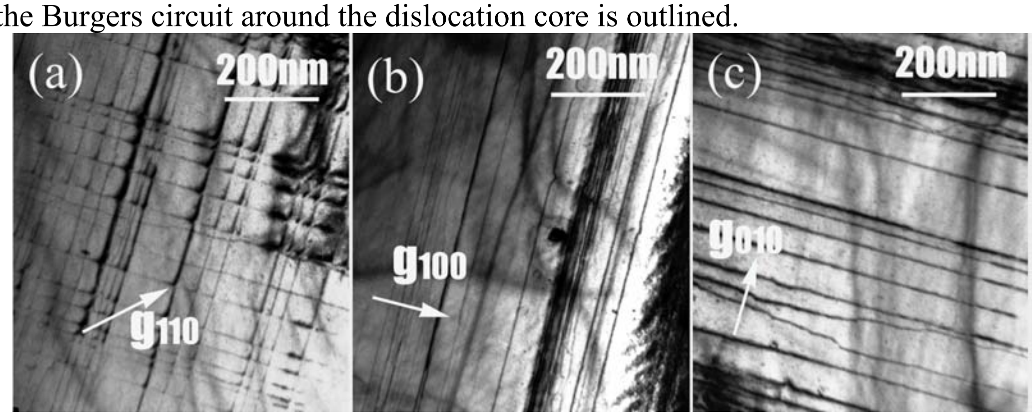

Fig.2 TEM bright images taken from a plan-view specimen under two-beam conditions showing some characteristics of the MDs. (a) When imaged with **g** = (110), two-set of dislocations were in contrast. (b) When imaged with **g** = (100), one of them was out of contrast and another set kept in contrast with the dislocation line along [010] direction. (c) When imaged with **g** = (010), the above dislocations were out of contrast, however, another set of dislocations were in contrast with the dislocation line along [100] direction.

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