

Microstructure and Defects of Co-Doped BaFe₂As₂ Single Crystal Thin Films

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Iron arsenide (FeAs) based superconductors have recently attracted great interest due to their high superconducting transition temperature (Tc) which can be as high as 56K. In order to achieve good superconducting properties in thin planar devices, the growth of high quality epitaxial films is necessary. There has been recent success growing epitaxial Co-doped BaFe₂As₂ (Ba-122) thin films on single crystal SrTiO₃ (STO) substrates but the STO conductivity due to oxygen vacancies is too large for accurate characterization. In this work we study Ba-122 films grown on insulating (La,Sr)(Al,Ta)O₃ (LSAT) substrates using thin epitaxial STO buffer layers.

Co-doped Ba-122 thin films were deposited on SrTiO₃-templated (001) LSAT substrate and bare perovskite single crystal substrates using pulsed laser deposition with a KrF ultraviolet excimer laser at 730-750 °C¹. Transmission electron microscopy (TEM) was performed using a JEOL 3011 and JEOL 2010F. Cross-sectional and Planar view TEM specimens were prepared by mechanical polishing and Ar-ion milling using a Gatan-PIPS.

The cross-sectional TEM bright field images of the films grown on bare LSAT (Fig. 1), 100 unit cell STO buffered LSAT (Fig. 2), 20 u.c. STO buffered LSAT (Fig. 3) and bare STO (Fig. 4) are shown. The corresponding selected-area electron diffraction (SAED) patterns from the Ba-122 layers are inset in the top right corner of each figure. The bright field image of the Ba-122 on bare STO (Fig. 1) shows many misoriented grains and the corresponding SAED pattern shows a typical polycrystalline pattern. The high-resolution TEM (HRTEM) image on the left side of Fig. 1 shows an example of high-angle grain boundaries in the Ba-122 film. The SAED patterns of the Ba-122 films on STO-templated LSAT and bare STO show the films are high quality epitaxial films. The bright field images in Fig. 2-4 show a high density of vertically aligned line defects in the Ba-122 films. The inset on the left side of Fig. 2 is a planar-view TEM dark field image of the Ba-122 films on 100 u.c. STO/LSAT. The uniformly distributed bright spots are vertically aligned defects visible in the cross-section TEM images. The HRTEM image on the left side of Fig.3 shows the interfacial structure between LSAT and 20 u.c. STO and between 20 u.c. STO and the Ba-122 film. The 2 nm disorder of atomic arrangement at the STO and Ba-122 interface shows weak bond at the interface or ion beam damage during TEM sample preparation.

In conclusion we find that BaFe₂As₂ superconducting thin films form a polycrystalline structure when grown on bare LSAT. However, the addition of a thin epitaxial SrTiO₃ buffer layer promotes the formation of a single crystal BaFe₂As₂ film. The use of oxide buffered growth to achieve high quality superconducting films greatly expands the range of viable substrates available for engineering and integration of these Ba-122 superconducting films.

References:

1. S. Lee et al., Template engineering of Co-doped BaFe₂As₂ single-crystal thin films. *Nature Materials*, in press.
2. The authors gratefully acknowledge the financial support through DOE grants DoE/BES DE-FG02-07ER46416 (X.Q.P) and the UM Electron Microbeam Analysis Lab.

Figure 1 – TEM micrographs of Ba-122 / LSAT . The inset on the left side shows high-angle grain boundary .

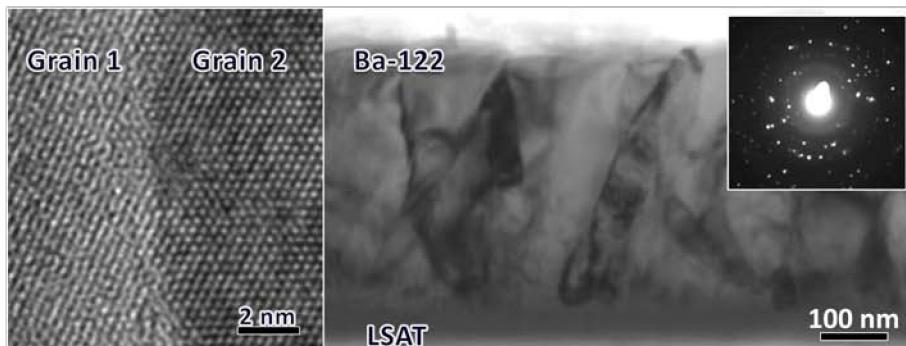


Figure 2 – TEM micrographs of Ba-122 / 100u.c. STO / LSAT. The inset on the left side is dark field planar-view image.

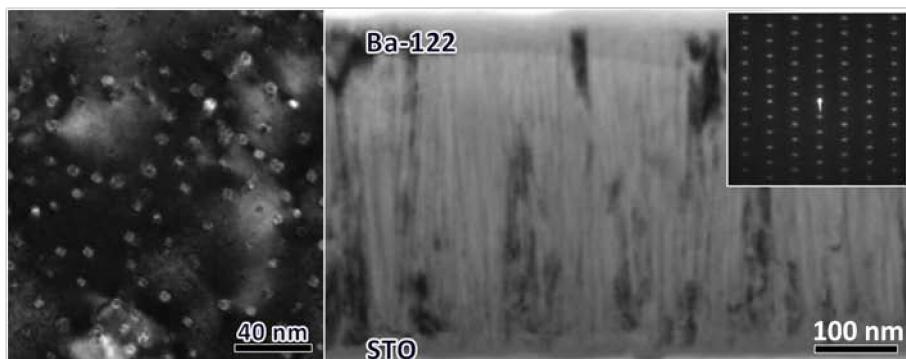


Figure 3 – TEM micrographs of Ba-122 / 20 u.c. STO / LSAT. The inset on the left side is HRTEM image of the interface structure.

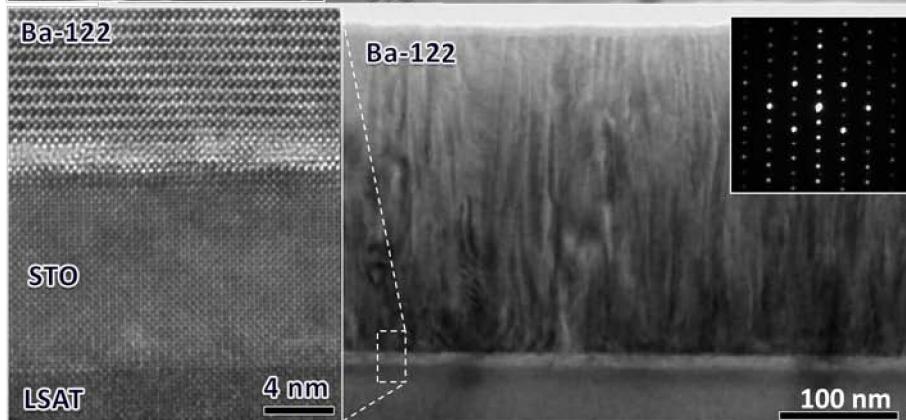


Figure 4 – TEM images of Ba-122 / STO.

