Characterization and investigation of Fe:STO thin films prepared by pulsed laser deposition

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Introduction

- Bulk SrTiO$_3$ well researched, defect model well known
- Conductivity of STO can be tailored by doping
- Effect of cation nonstoichiometry on (electrical) properties not so well researched
- Aim: linking stoichiometry, structure and properties of Fe:SrTiO$_3$
Sample preparation via PLD

Deposition parameters
Standard: 400 mJ set, 650 °C, 0.15 mbar O₂; 5 Hz

Variation of laser fluence and repetition rate for stoichiometric targets

SrTi$_{0.98}$Fe$_{0.02}$O$_3$

Stoichiometric target

Sr overstoichiometric target

Sr excess in targets:
3 % Sr
5 % Sr
7 % Sr
11 % Sr

Substrates:
Electrical measurements: Nb:STO
XRD (reciprocal space map): STO
XRD (thin film gracing incidence): MgO
ICP-OES: MgO

ICP-OES: MgO
X-ray diffraction of targets

Overstoichiometric targets: Solid state route pressing, then
1) 1000 °C, 2 h
2) 1200 °C, 4 h remilling and pressing
3) 1400 °C, 4.5 h

Sr-rich phases are present even after three sintering steps.

With Sr overstoichiometry

7% Sr excess

Sr3Ti2O7
SrTiO3

sintering step 1
sintering step 2
sintering step 3

Sr-rich phases are present even after three sintering steps.
X-ray diffraction of targets

Overstoichiometric targets:
Solid state route pressing, then
1) 1000 °C, 2 h
2) 1200 °C, 4 h remilling and pressing
3) 1400 °C, 4.5 h

Thin films are phase pure
Chemical analysis of thin films (ICP-OES)

Deposited from a stoichiometric target

Sr excess in the target
Chemical analysis of thin films (ICP-OES)

Deposited from a stoichiometric target

Sr excess in the target
X-ray diffraction of thin films

Stoichiometry variation

Fluence variation (5 Hz)

Fluence variation (1 Hz)

Frequency variation

Thin films deposited on STO substrates (=reference)

Deposited from Sr overstoichiometric targets

Deposited from stoichiometric targets
Conductivity measurements

By means of Electrochemical Impedance Spectroscopy

Nyquist Plot 300 °C
Conductivity
Conductivity
Conductivity

\[ \log \left( \frac{\sigma}{\text{Scm}^{-1}} \right) \]

against

\[ \frac{1000}{T} \text{ [1/K]} \]

for pellet and thin film.
Conductivity
Conductivity
Conductivity

\[ \log(\sigma / \text{Scm}^{-1}) \] vs. \[ 1000/T \text{ [1/K]} \]

- pellet
- 5% Sr
- 7% Sr
- 200 mJ
- 300 mJ
- 3% Sr excess in target
- thin film, 400 mJ
Conductivity
Structure vs. Conductivity

Structure and conductivity for thin films deposited from targets with a Sr overstoichiometry.
Model

\[ \text{Sr}^{2+}, \text{Ti}^{4+} / \text{Fe}^{3+}, \text{O}^{2-}, V'_{\text{Sr}} \]

\[ \text{CB} \]

\[ \text{Fe'}_{\text{Ti}} \]

\[ E_F \]

\[ \text{VB} \]

\[ \text{CB} \]

\[ \text{Fe}^*_{\text{Sr}} \]

\[ E_F \]

\[ \text{Fe'}_{\text{Ti}} \]

\[ \text{VB} \]
Model

Discussion

1. ICP-OES

Fe:STO with Sr excess:

2. XRD

3. Band model

4. Charge carrier concentration

5. $\sigma$

3. Structure

Composition

Properties

Discussion

Fe:STO with Sr excess:

0 %

7 %
Thank you for your attention!