Effect of the substrate temperature on the properties of Nb-doped TiO_2 thin films deposited by magnetron sputtering

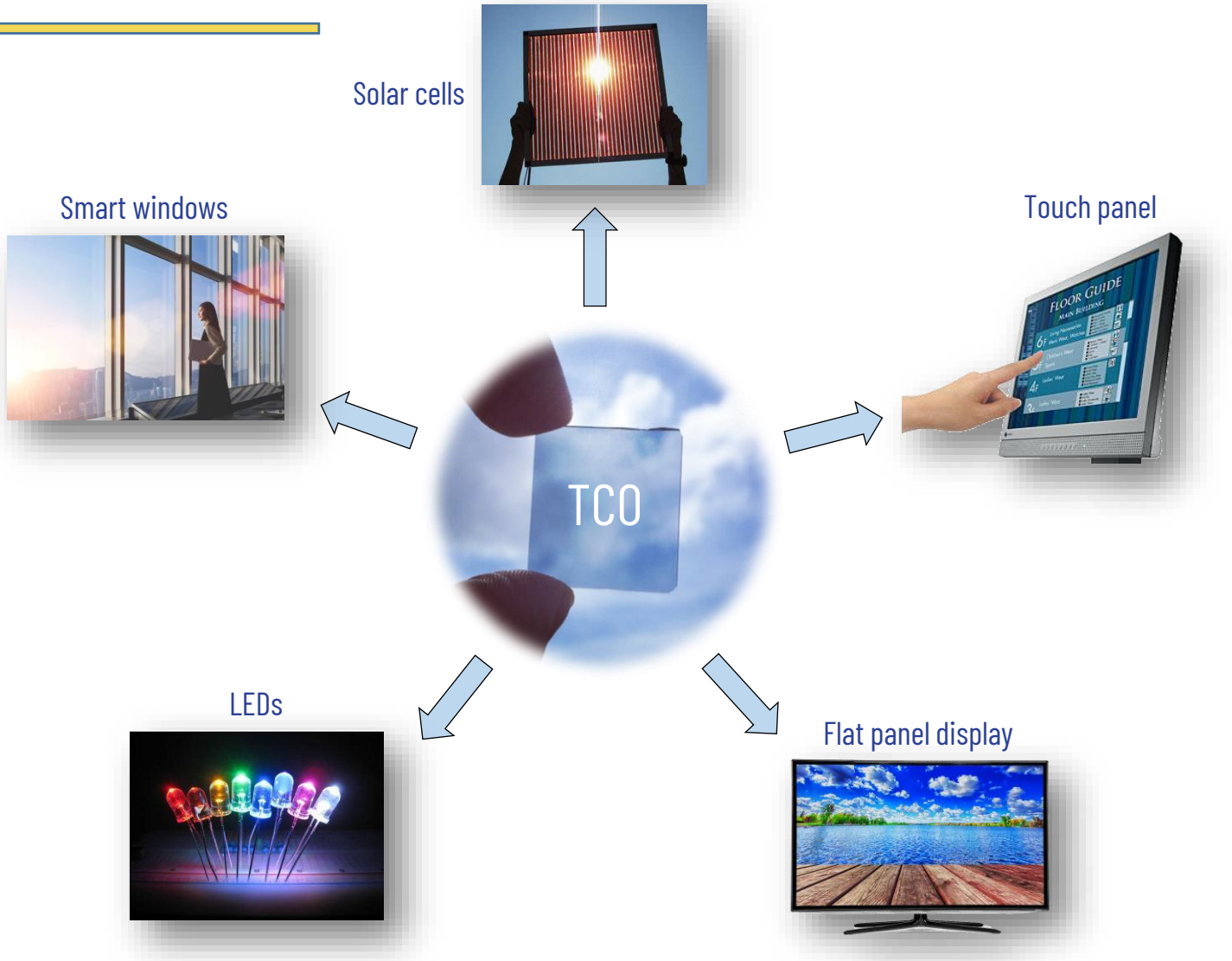
Francisco Alfaro[1], Rafael G. Delatorre[1], Julio C. Sagás[2] and Diego A. Duarte[1]

[1] Joinville Center of Technology, Federal University of Santa Catarina, Brazil
[2] Center of Technological Sciences, Santa Catarina State University, Brazil.

SUMMARY

INTRODUCTION

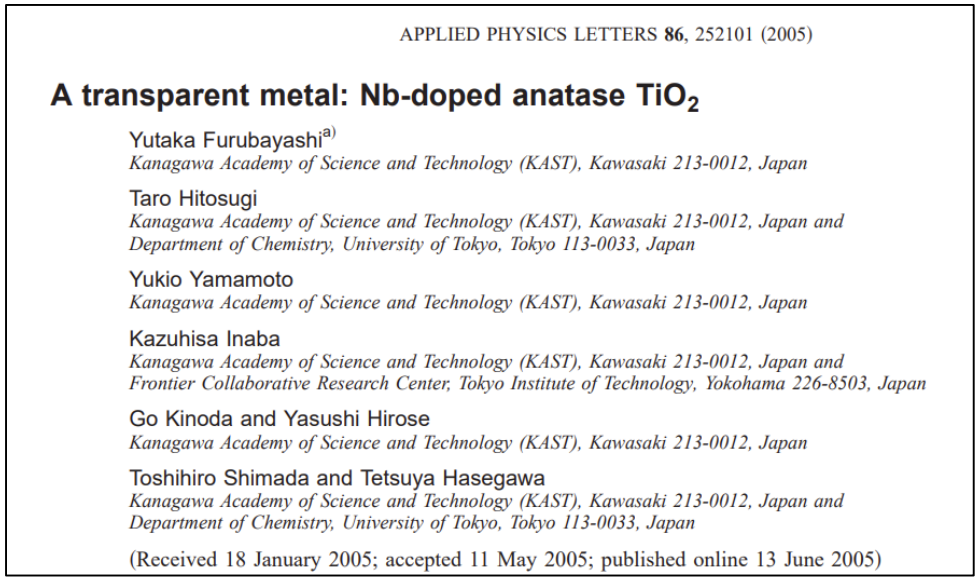
Transparent conducting oxides (TCOs)



INTRODUCTION

Nb:TiO_2 thin films as TCOs

- High cost of comercial TCOs (ITO: indium tin oxide)
- Alternative materials:



APPLIED PHYSICS LETTERS **86**, 252101 (2005)

A transparent metal: Nb-doped anatase TiO_2

Yutaka Furubayashi[a)]
Kanagawa Academy of Science and Technology (KAST), Kawasaki 213-0012, Japan

Taro Hitosugi
Kanagawa Academy of Science and Technology (KAST), Kawasaki 213-0012, Japan and Department of Chemistry, University of Tokyo, Tokyo 113-0033, Japan

Yukio Yamamoto
Kanagawa Academy of Science and Technology (KAST), Kawasaki 213-0012, Japan

Kazuhisa Inaba
Kanagawa Academy of Science and Technology (KAST), Kawasaki 213-0012, Japan and Frontier Collaborative Research Center, Tokyo Institute of Technology, Yokohama 226-8503, Japan

Go Kinoda and Yasushi Hirose
Kanagawa Academy of Science and Technology (KAST), Kawasaki 213-0012, Japan

Toshihiro Shimada and Tetsuya Hasegawa
Kanagawa Academy of Science and Technology (KAST), Kawasaki 213-0012, Japan and Department of Chemistry, University of Tokyo, Tokyo 113-0033, Japan

(Received 18 January 2005; accepted 11 May 2005; published online 13 June 2005)

Target

- $T > 80\%$
- $\rho < 10^{-3}\ \Omega\cdot$cm

- Brazil is the largest producer of TiO_2 in Latin America (~ 1% of the world's production) and the largest producer of Nb in the world, with ~ 90% of the world's resources.

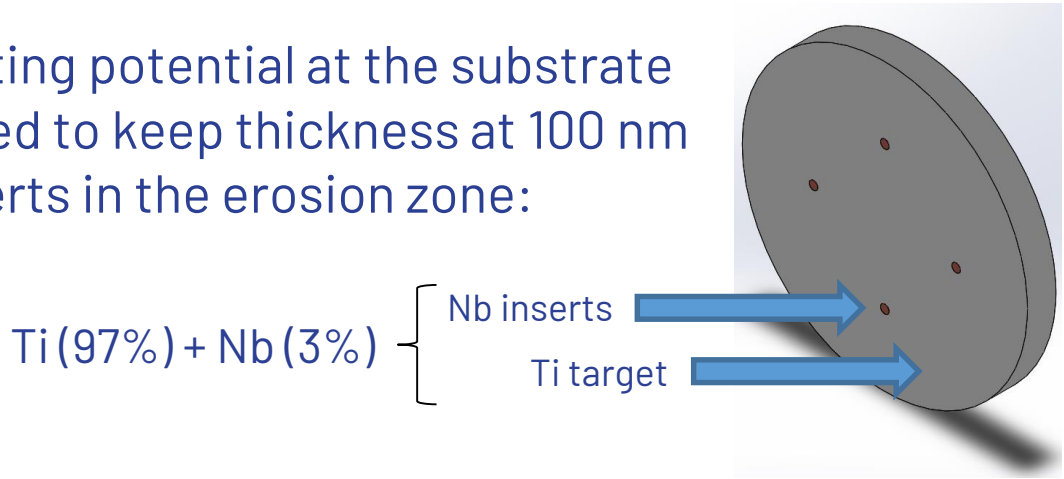
EXPERIMENTAL SETUP

Nb:TiO_2 thin films

- Depositions were made in glass by magnetron sputtering with the following experimental parameters:

Sample	***T*** (°C)	***I*** (A)	***P*** (kW)	Gas flow rate (sccm)		***p*** (mtorr)
				Ar	O_2	
TiO_2	300	2.0	1.0	1.5	4.4	6.0
Nb:TiO_2	room	2.0	1.0	1.5	4.4	6.0
Nb:TiO_2	300	2.0	1.0	1.5	4.4	6.0

- Depositions made with floating potential at the substrate
- Deposition time was adjusted to keep thickness at 100 nm
- One target with four Nb inserts in the erosion zone:



EXPERIMENTAL SETUP

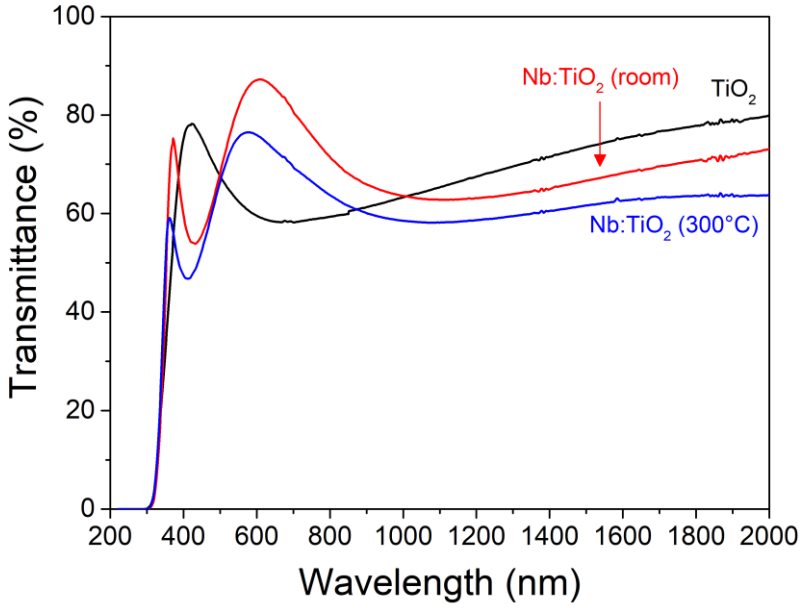
Nb:TiO_2 thin films

- After depositions, films were evaluated by:

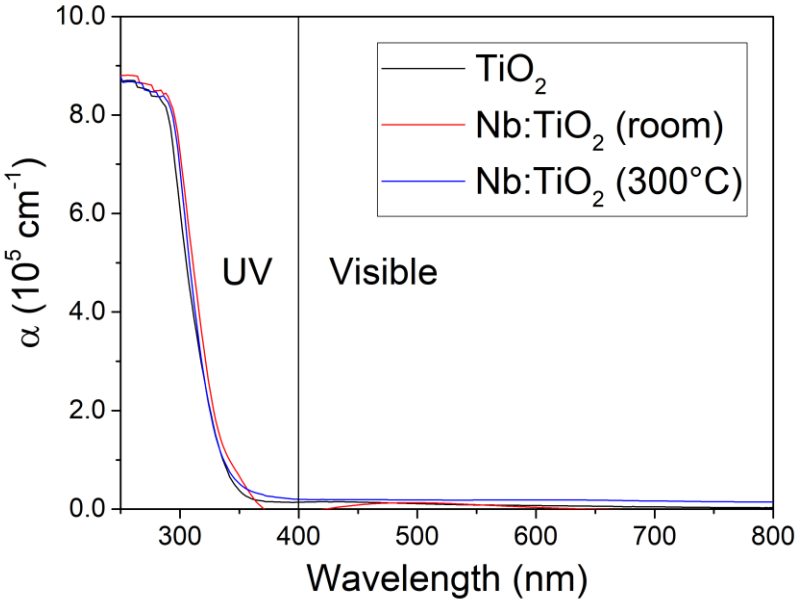
- Optical spectrophotometry
- Mechanical profilometry (to evaluate the thickness of 100 nm)
- Four point probes
- X-ray diffraction
- X-ray photoelectron spectroscopy

RESULTS AND DISCUSSIONS

Optical spectrophotometry



Cut-off wavelenght in the UV region!



Sample	T_{av}(%)	E_g(eV)
TiO_2(300°C)	69.0	3.4
Nb:TiO_2(room)	68.9	3.3
Nb:TiO_2(300°C)	62.5	3.5

- Nb do not changes the optical gap;
- Vacuum annealing decreases the average transmittance.

RESULTS AND DISCUSSIONS

Four point probes

Nb incorporation decreased **one** order of magnitude.

Sample	ρ (Ω·cm)
TiO_2 (300°C)	$5.7 \cdot 10^{3}$
Nb:TiO_2 (room)	$2.7 \cdot 10^{2}$
Nb:TiO_2 (300°C)	$2.8 \cdot 10^{-2}$

RESULTS AND DISCUSSIONS

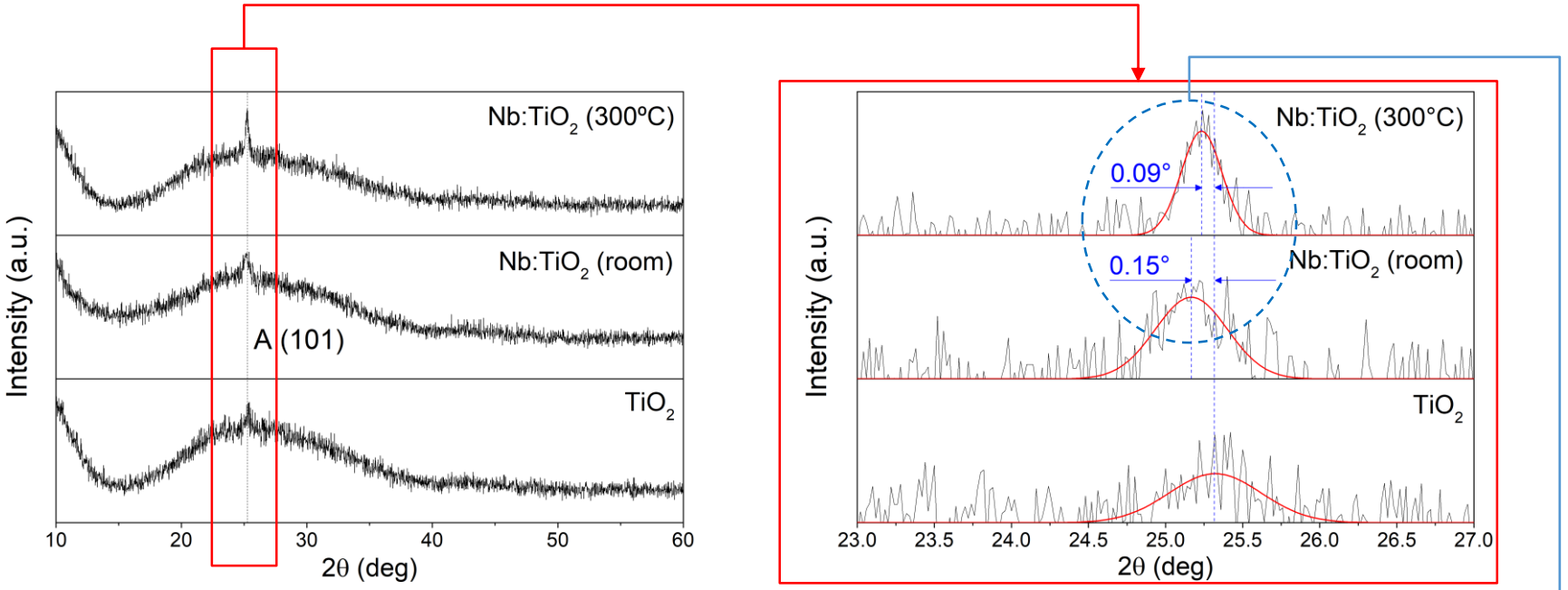
Four point probes

Sample	ρ (Ω·cm)
TiO_2 (300°C)	$5.7 \cdot 10^{3}$
Nb:TiO_2 (room)	$2.7 \cdot 10^{2}$
Nb:TiO_2 (300°C)	$2.8 \cdot 10^{-2}$

Nb incorporation combined with vacuum annealing decreased **five** orders of magnitude (synergistic effect).

RESULTS AND DISCUSSIONS

X-ray diffraction



Sample	2θ (deg)	FWHM (deg)	Crystallite size (nm)
TiO_2 (300°C)	25.55	0.70	12.2
Nb:TiO_2 (room)	25.17	0.55	15.5
Nb:TiO_2 (300°C)	25.23	0.31	27.4

- Shift to lower angles means that the crystal lattice has increased.

RESULTS AND DISCUSSIONS

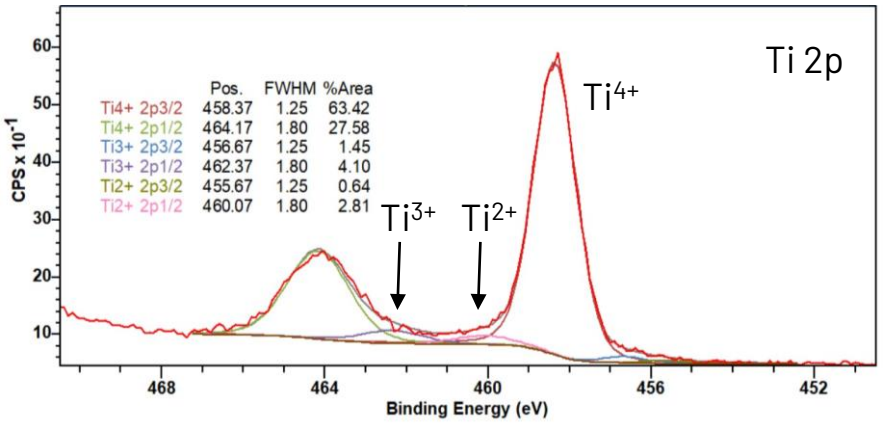
X-ray photoelectron spectroscopy

- Ti^{4+}: titanium dioxide (TiO_2)
- Ti^{3+}: suboxide (eg.: Ti_2O_3)
- Ti^{2+}: suboxide (eg.: TiO)

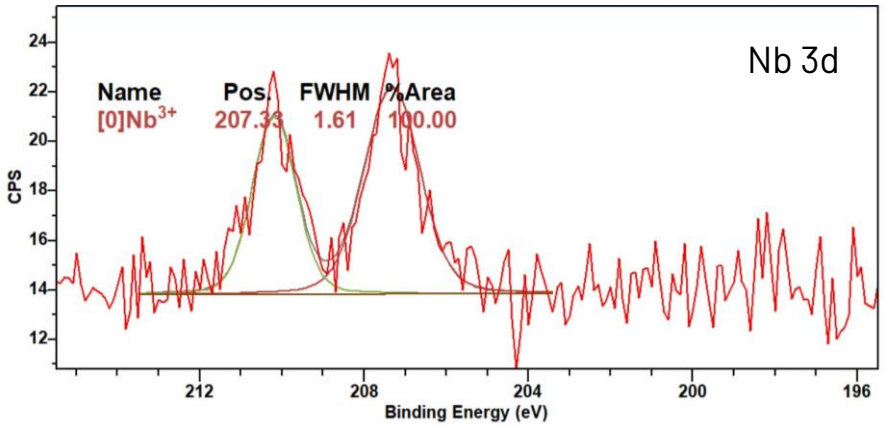
- Normalized with respect to the amount of Ti in each sample.

Sample	Nb (%)	Ti (%)		
		Ti^{4+}	Ti^{3+}	Ti^{2+}
TiO_2 (300°C)	0.0	95.9	4.1	0.0
Nb:TiO_2 (room)	0.1	95.4	4.2	0.4
Nb:TiO_2 (300°C)	0.3	91.0	5.6	3.4

Nb:TiO_2 (300°C)



Nb:TiO_2 (300°C)



RESULTS AND DISCUSSIONS

X-ray photoelectron spectroscopy

Sample	Nb (%)	Ti (%)		
		Ti^{4+}	Ti^{3+}	Ti^{2+}
TiO_2 (300°C)	0.0	95.9	4.1	0.0
Nb:TiO_2 (room)	0.1	95.4	4.2	0.4
Nb:TiO_2 (300°C)	0.3	91.0	5.6	3.4

- The addition of Nb increase surface defects (oxygen deficiency).

- Ti^{4+}: titanium dioxide (TiO_2)
- Ti^{3+}: suboxide (eg.: Ti_2O_3)
- Ti^{2+}: suboxide (eg.: TiO)

RESULTS AND DISCUSSIONS

X-ray photoelectron spectroscopy

Sample	Nb (%)	Ti (%)		
		Ti^{4+}	Ti^{3+}	Ti^{2+}
TiO_2 (300°C)	0.0	95.9	4.1	0.0
Nb:TiO_2 (room)	0.1	95.4	4.2	0.4
Nb:TiO_2 (300°C)	0.3	91.0	5.6	3.4

- Vacuum annealing improve surface defects (oxygen deficiency)

- Ti^{4+}: titanium dioxide (TiO_2)
- Ti^{3+}: suboxide (eg.: Ti_2O_3)
- Ti^{2+}: suboxide (eg.: TiO)

RESULTS AND DISCUSSIONS

X-ray photoelectron spectroscopy

Sample	Nb (%)	Ti (%)		
		Ti^{4+}	Ti^{3+}	Ti^{2+}
TiO_2 (300°C)	0.0	95.9	4.1	0.0
Nb:TiO_2 (room)	0.1	95.4	4.2	0.4
Nb:TiO_2 (300°C)	0.3	91.0	5.6	3.4

- Sample produced with vacuum annealing presented higher Nb concentration.

- Ti^{4+}: titanium dioxide (TiO_2)
- Ti^{3+}: suboxide (eg.: Ti_2O_3)
- Ti^{2+}: suboxide (eg.: TiO)

FINAL REMARKS

- The incorporation of Nb do not changes the optical transmittance of TiO_2 thin films;
- Nb decreases the electrical resistivity of TiO_2 thin films;
- Nb increases the lattice constants and surface defects;
- Deposition of Nb:TiO_2 with heated substrate promotes a synergistic effect able to reduce the electrical resistivity near to that obtained with comercial TCOs with the optical transmittance similar to TiO_2.
- NEXT STEPS: produce thinner layers with higher Nb concentration (~ 3%).

ACKNOWLEDGMENTS

406376/2022-0
307408/2021-3

Thank you!

Diego A. Duarte
diego.duarte@ufsc.br
https://lats.ufsc.br