A new strategy for optimizing the microstructure and giant dielectric properties of TiO_2 *via* acceptor/donor ratio tuning

Wattana Tuichai[a], Jurimart Wongsricha[a], Nutthakritta Phromviyo[b], Bundit Putasaeng[c], Supamas Danwittayakul[c], Pornjuk Srepusharawoot[a,b], and Prasit Thongbai[a,b,*]

[1]*Giant Dielectric and Computational Design Research Group (GD–CDR), Department of Physics, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand*

[2]*Institute of Nanomaterials Research and Innovation for Energy (IN–RIE), Khon Kaen University, Khon Kaen 40002, Thailand*

[3]*National Metal and Materials Technology Center, 114 Thailand Science Park, Paholyothin Road, Klong 1, Klong Luang, Pathumthani 12120, Thailand*

*E–mail address: pthongbai@kku.ac.th (P. Thongbai)

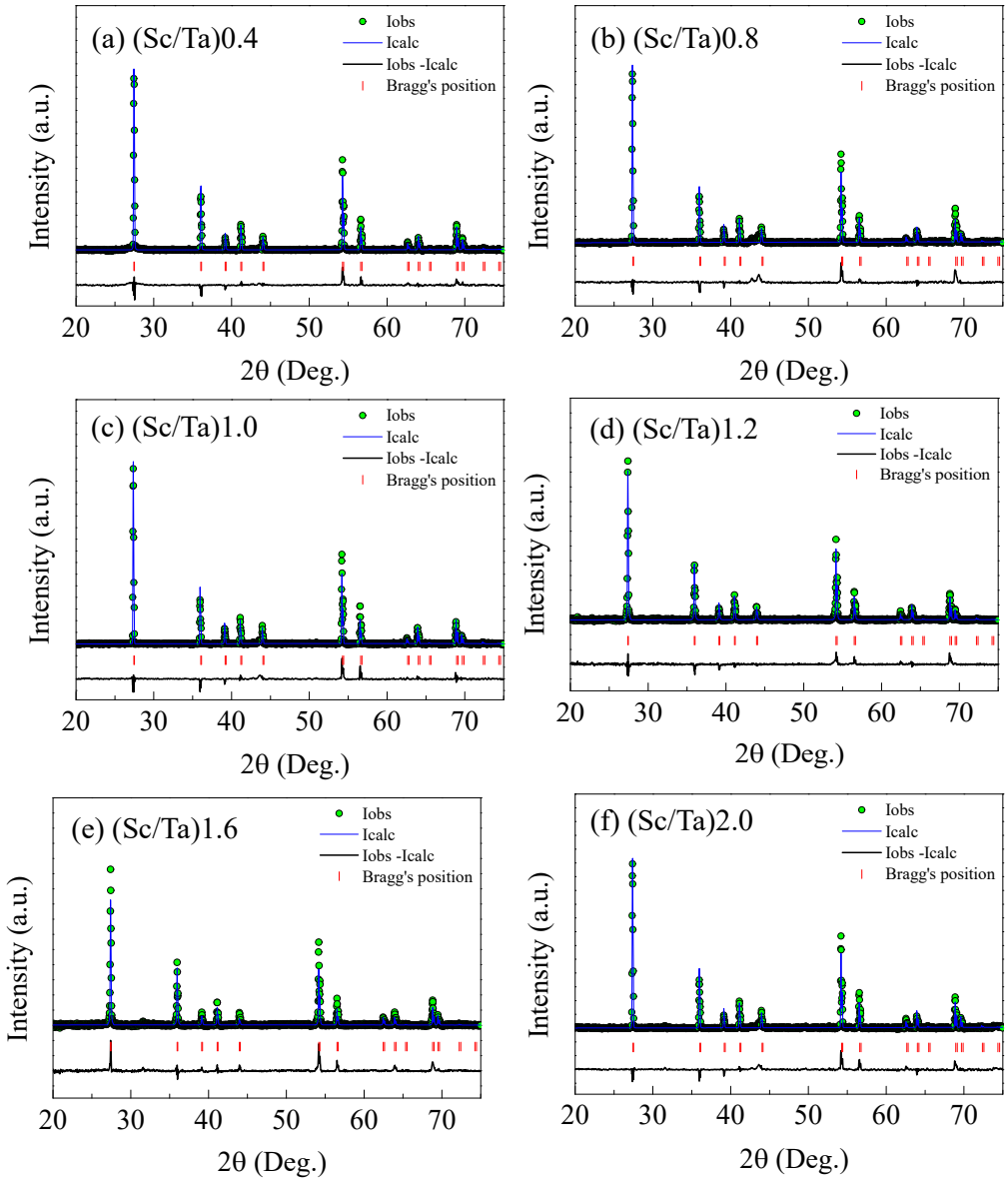

Fig. S1 Rietveld refinements for ScTa–TO ceramics with Sc^{3+}/Ta^{5+} ratios of (a) 0.4, (b) 0.8, (c) 1.0, (d) 1.2, (e) 1.6, and (f) 2.0.

Table S1 Lattice parameters and density of ScTa–TO ceramics with Sc^{3+}/Ta^{5+} ratios of 1.2 and 1.6.

Sample	(Sc/Ta)1.2	(Sc/Ta)1.6
$a = b$ (Å)	4.604	4.603
c (Å)	2.972	2.972
V $(Å)^3$	62.995	62.962
R_{exp}(%)	4.322	5.927
R_p(%)	3.541	3.923
R_{wp}(%)	5.280	6.159
χ^2	1.492	1.080
ρ (%)	4.36	4.42
Bond length (Å)		
$[\mathbf{A}–O]_1$	1.954	1.953
$[\mathbf{A}–O]_2$	1.987	1.987
$[\mathbf{A}–O]_3$	3.494	3.493
$\mathbf{A}_{(0,0,0)}$–$\mathbf{A}_{(0,0,1)}$	2.972	2.972

$[A–O]_1 = A_{(0,0,0)}–O_{(0.19480,-0.19480,0.50000)}$

$[A–O]_2 = A_{(0,0,0)}–O_{(0.30520,0.30520,0.00000)}$

$[A–O]_3 = A_{(0,0,0)}–O_{(0.30520,-0.69480,0.00000)}$

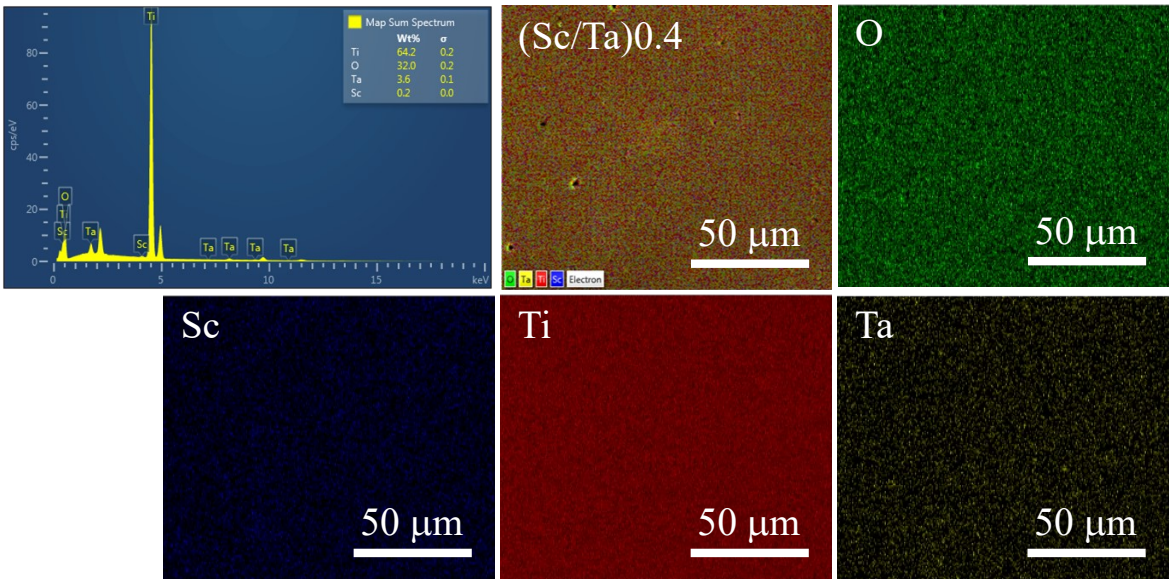

Fig. S2 EDS spectrum and SEM–mapping images of (Sc/Ta)0.4 ceramic.

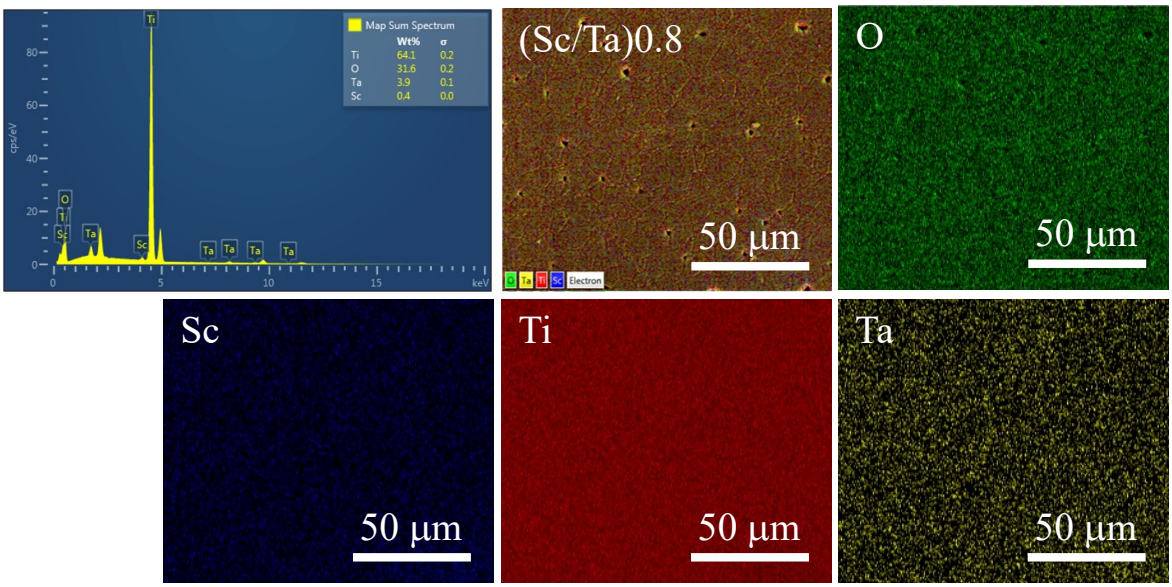

Fig. S3 EDS spectrum and SEM–mapping images of (Sc/Ta)0.8 ceramic.

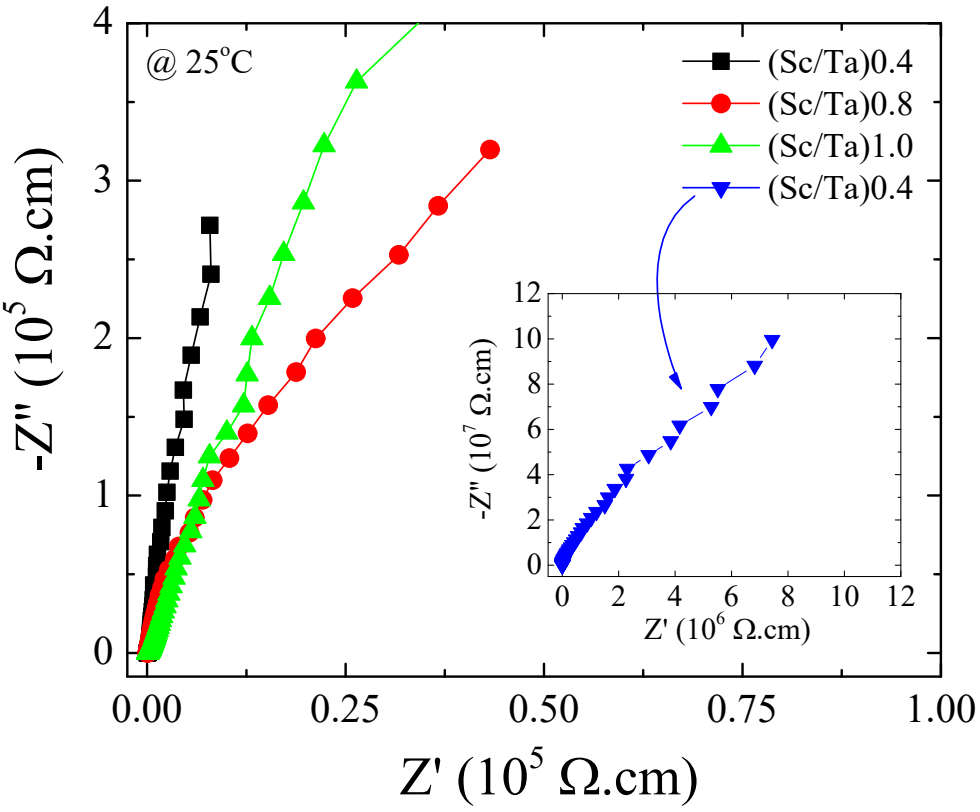

Fig. S4 Z* plots at 25 °C for ScTa–TO ceramics with Sc^{3+}/Ta^{5+} ratios of 0.4, 0.8, and 1.0; inset shows Z* plots at 25 °C for ScTa–TO ceramic with Sc^{3+}/Ta^{5+} ratio of 2.0.