Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Defect Generation in TiO_2 Nanotube Anodes via Heat Treatment in Various Atmospheres for Lithium-Ion Batteries

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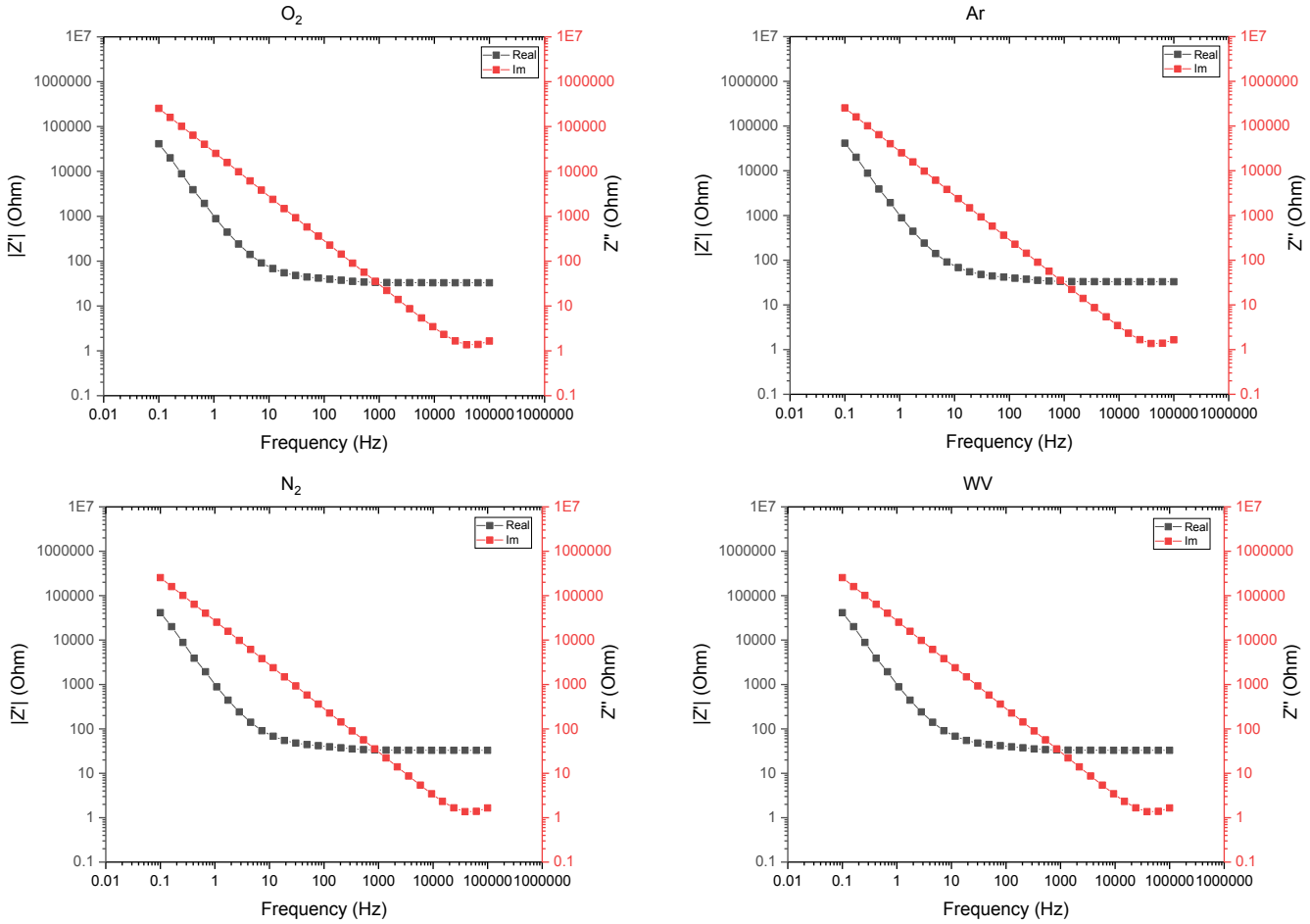

Figure S1. Bode plots of anatase TiO_2 nanotubes annealed in various atmospheres.

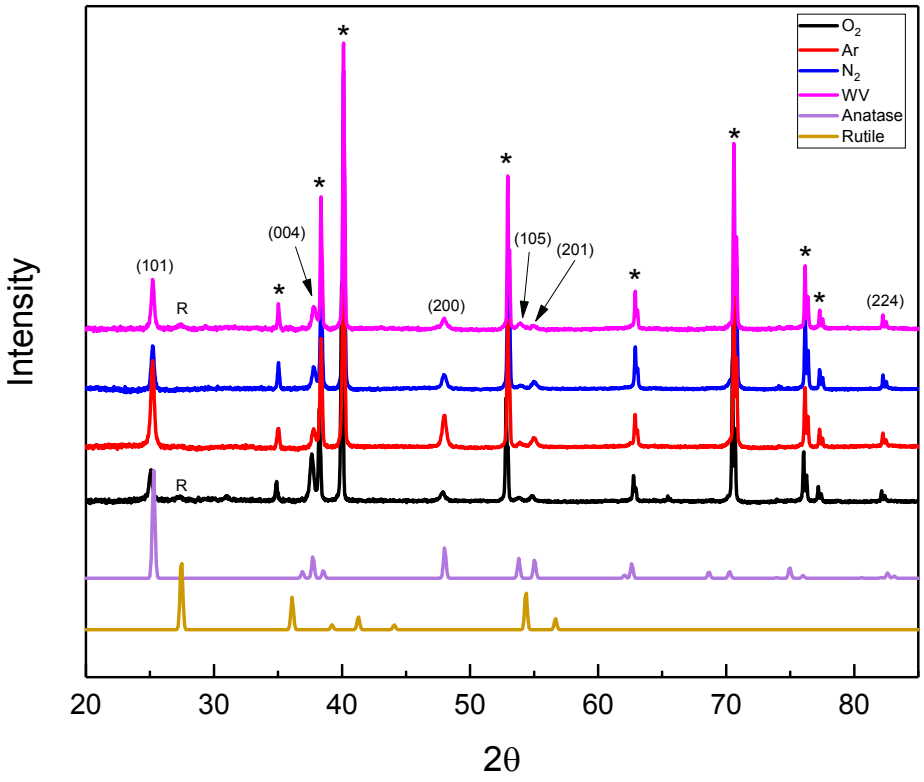

Figure S2. XRD spectra of anatase TiO_2 nanotubes annealed in different atmospheres. R indicates rutile (110) peak. * indicates metallic Ti.

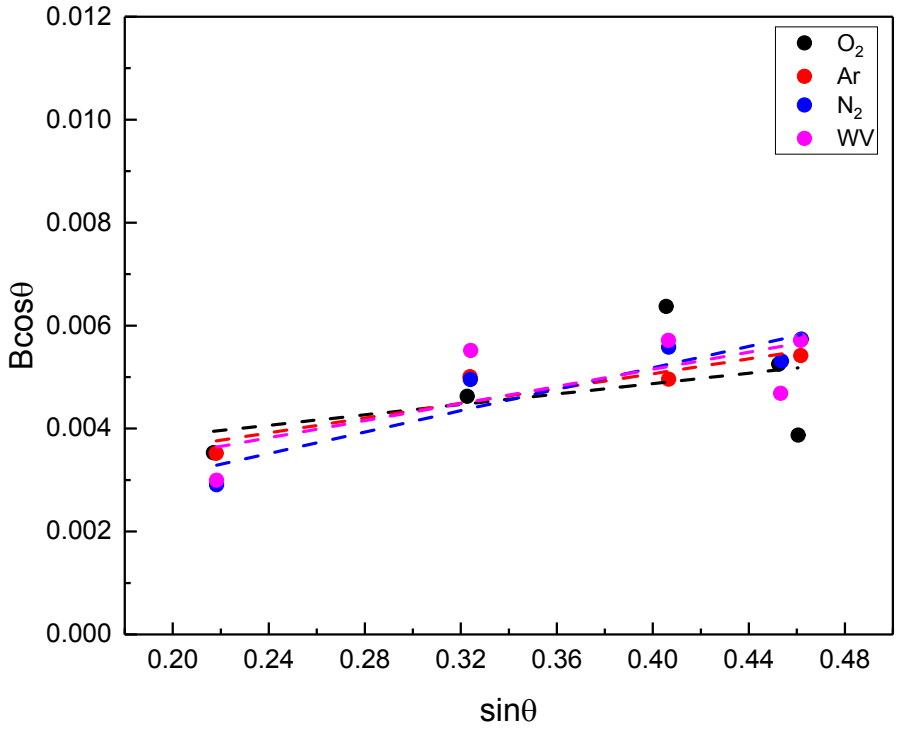

Figure S3. Williamson-Hall plots of anatase TiO_2 nanotubes annealed in different atmospheres.

Scherrer Equation: $$L = \frac{K\lambda}{B\cos\theta}$$ (S1)

L	Crystallite size
K	Shape factor
λ	Wavelength
B	FWHM
θ	Measurement angle
ε	Strain

Williamson-Hall Equation: $$B\cos\theta = 4\epsilon\sin\theta + \frac{K\lambda}{L}$$ (S2)

Atmosphere	**O_2**	**Ar**	**N_2**	**WV**
Slope	0.00506	0.00718	0.01041	0.00831
Strain (%)	0.001265	0.001795	0.0026025	0.0020775
Crystallite Size (nm)	39	39	48	46

Table S1. Slope and strain values obtained from Williamson-Hall plots of anatase TiO_2 nanotubes annealed in different atmospheres. Crystallite size for each sample was calculated using the Scherrer equation.

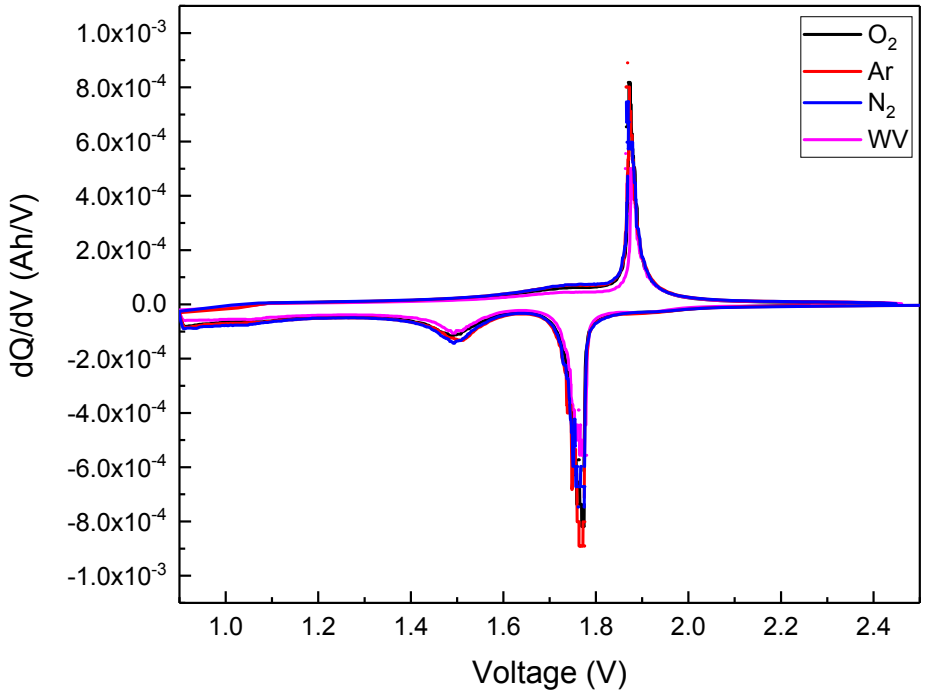

Figure S4. 1st cycle dQ/dV plots of anatase TiO_2 nanotubes annealed in different atmospheres.

Two-point Conductivity

$$R = \rho * \frac{l}{s} \quad \text{(S3)}$$

$$s = \pi r^2 * F \quad \text{(S4)}$$

$$P = 1 - \frac{2\pi * w * (w + D)}{\left(\sqrt{3} * (D + 2w)^2\right)} \quad \text{(S5)}$$

R	Resistance
l	Tube length
F	Effective factor
P	Porosity
w	Tube wall thickness
D	Tube diameter
r	Contact radius
ρ	Resistivity

Electrochemical Impedance Spectroscopy

$$D_{Li} = \frac{R^2T^2}{2C_{Li}^2\sigma^2n^4F^4A^2} \quad \text{(S6)}$$

R	Gas constant
T	Temperature
F	Faraday's Constant
A	Geometric surface area
C_{Li}	Lithium concentration
D_{Li}	Diffusion coefficient
σ	Warburg factor
n	Transferred charge