Mixed phase Ti^{3+}-rich TiO_2 thin films by oxide defect engineered crystallization

Supplementary information

Lauri Palmolahti[1], Harri Ali-Löytty[1,2*], Markku Hannula[1], Tuomas Tinus[1], Kalle Lehtola[1], Antti Tukiainen[3], Jarno Reuna[3], and Mika Valden[1*]

[1]Surface Science Laboratory, Physics Unit, Faculty of Engineering and Natural Sciences, Tampere University, Tampere, Finland

[2]Liquid Sun Ltd., Tampere, Finland

[3]Faculty of Engineering and Natural Sciences, Tampere University, Tampere, Finland

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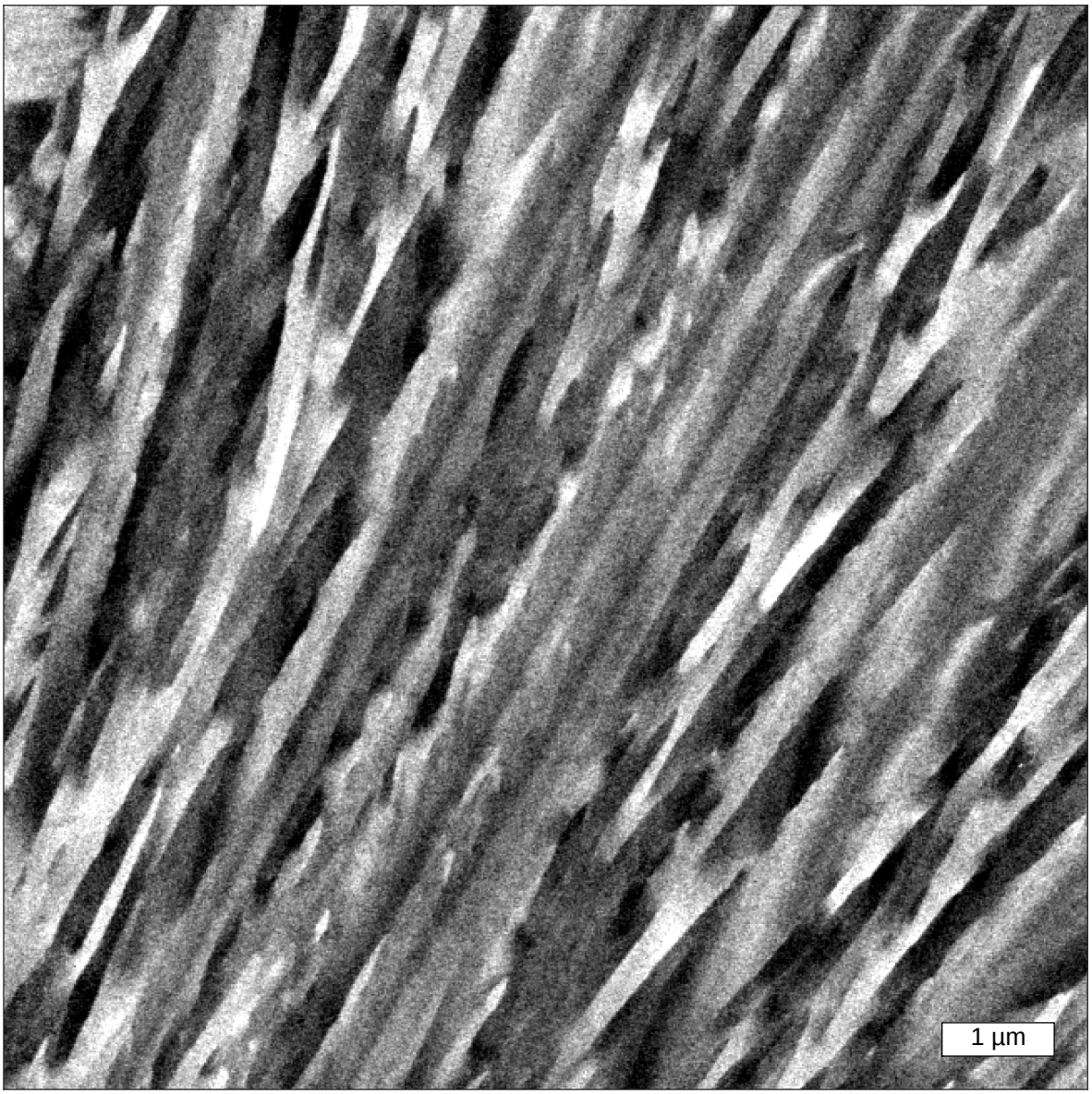

Fig. S1: SEM image of TiO_2-40 sample after vacuum annealing at 500 °C.

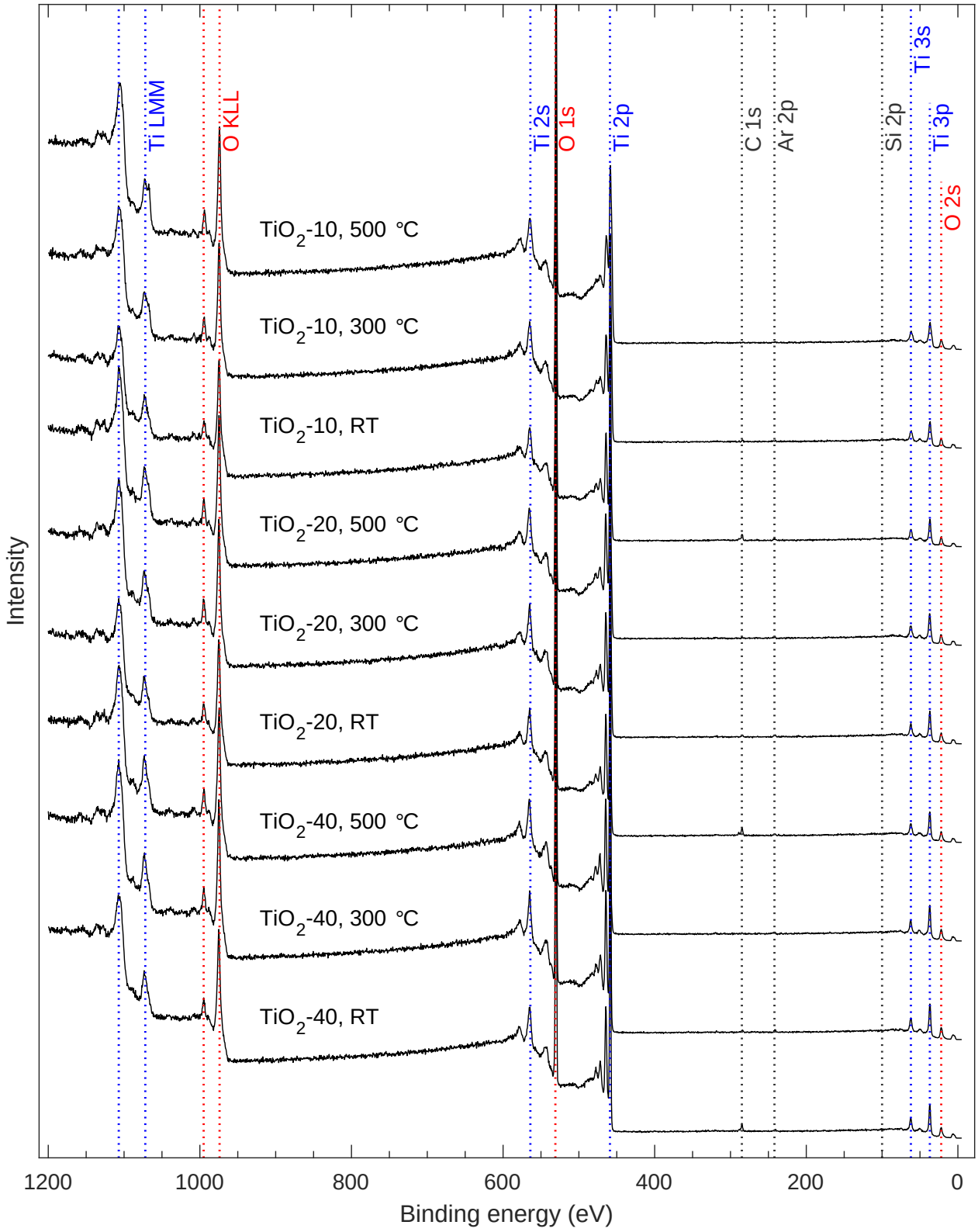

Fig. S2: XPS survey spectra from the cumulative vacuum annealing series using Al Kα radiation ($E_p = 1486.6$ eV).

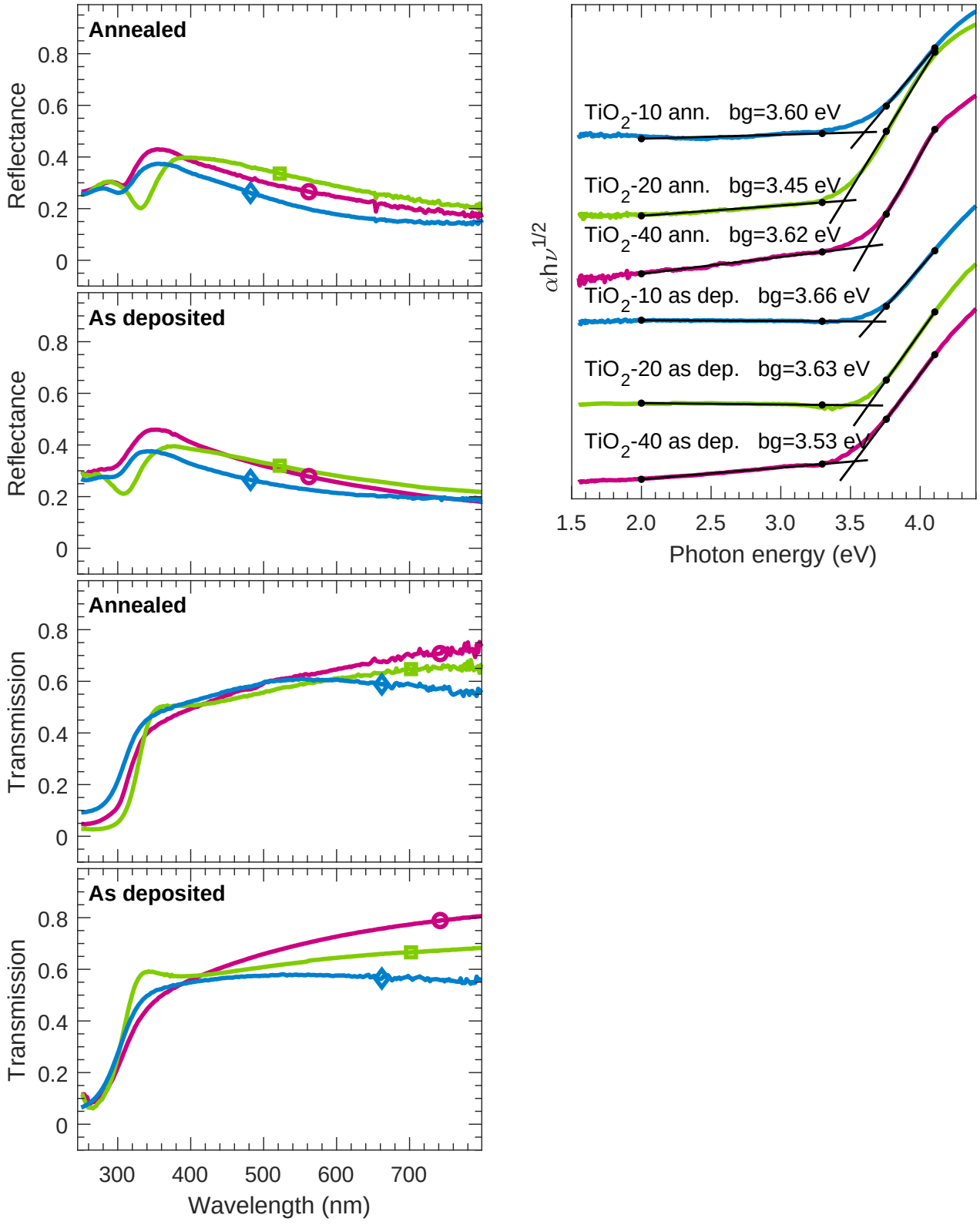

Fig. S3: Transmission and reflectance spectra of as deposited and 500 °C vacuum annealed samples (left) and Tauc plots calculated from the transmission and reflectance spectra (right). Two lines were fitted to the Tauc plot, one to the background before the edge and the second one to the absorption edge. The band-gap values were calculated from the intersection points of these two lines. The black dots represent the energy range where the lines were fitted.

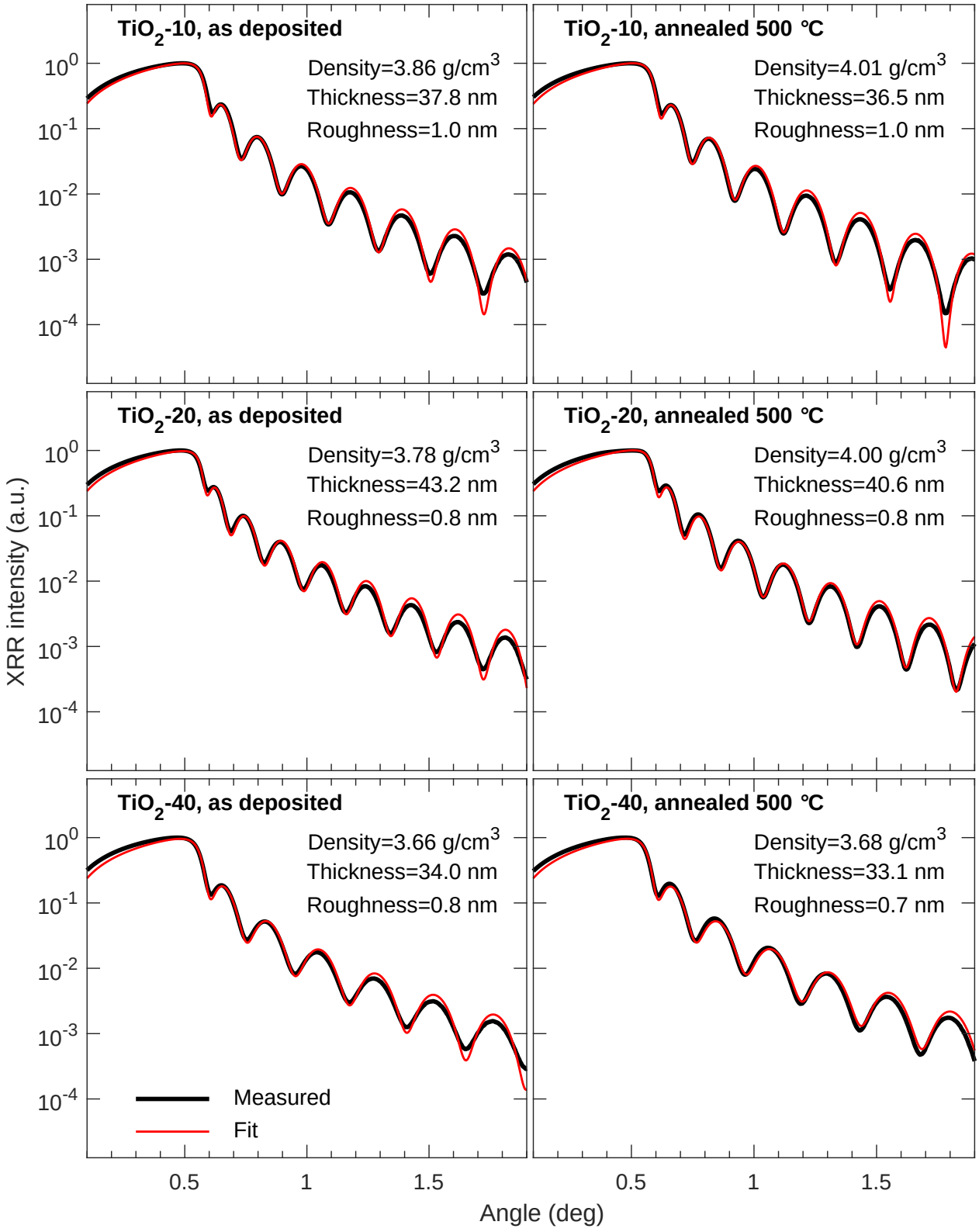

Fig. S4: X-ray reflection of as deposited samples and samples vacuum annealed at 500 °C (black line). The data was fitted with a model of TiO_2–SiO_2–Si layer structure (red line).

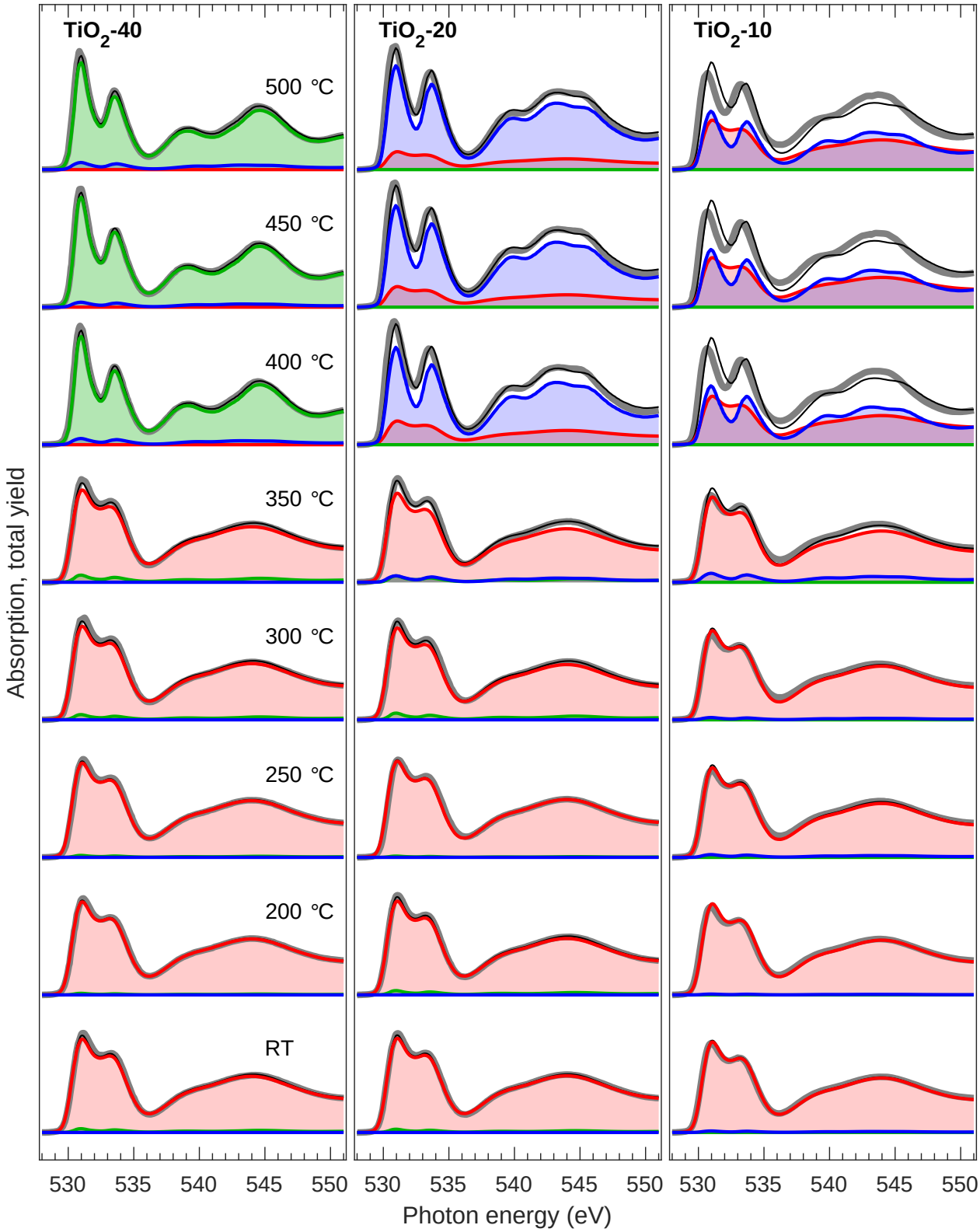

Fig. S5: X-ray absorption total electron yield spectra of O K-edge from the cumulative vacuum annealing series. The thick gray line represents the measured data. The spectra were fitted with amorphous (red), anatase (green) and rutile (blue) reference spectra and the thin black line is the sum of the fitted components.

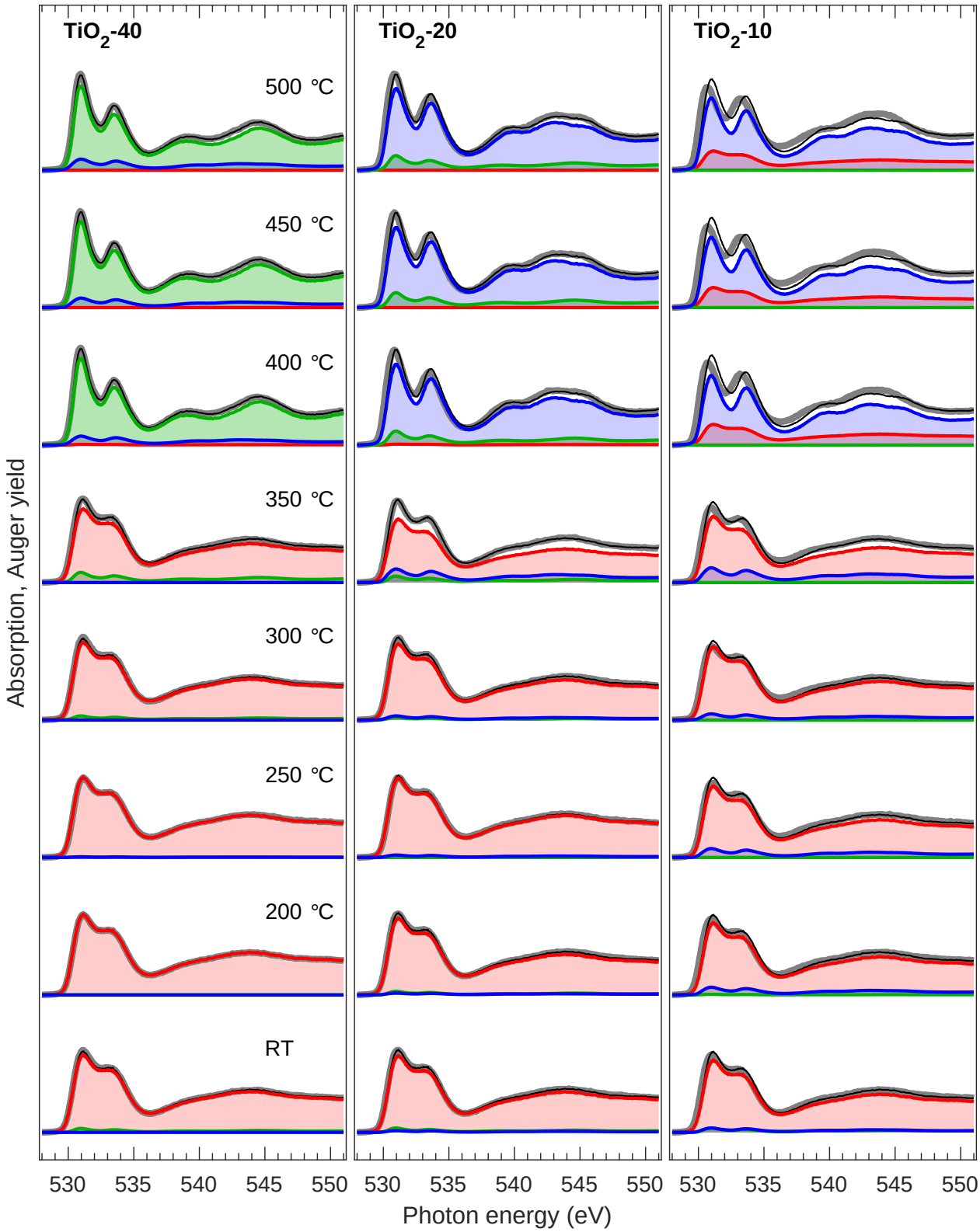

Fig. S6: X-ray absorption Auger electron yield spectra of O K-edge measured from the cumulative vacuum annealing series. The thick gray line represents the measured data. The spectra were fitted with amorphous (red), anatase (green) and rutile (blue) reference spectra and the thin black line is the sum of the fitted components.

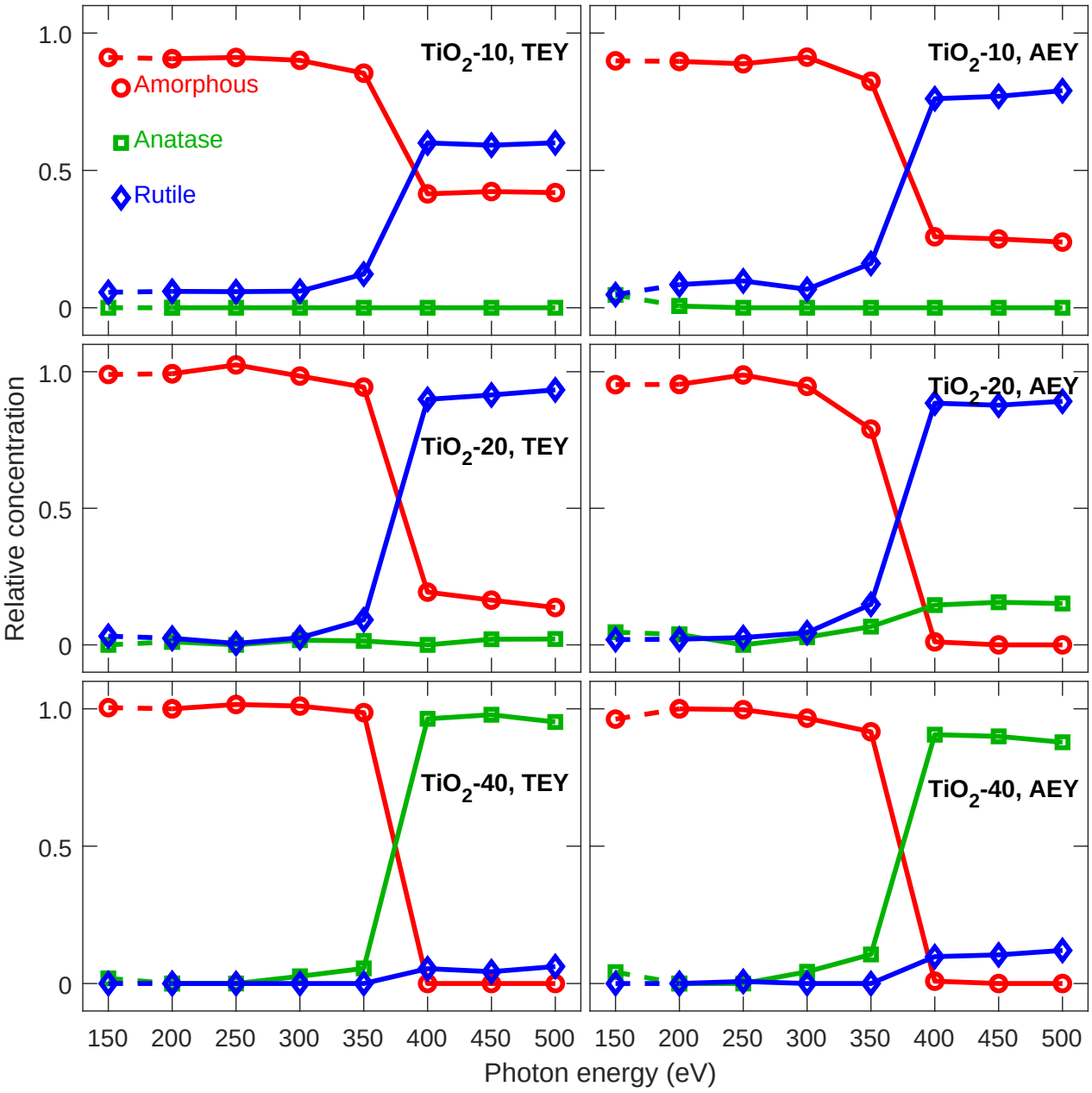

Fig. S7: Relative concentrations of amorphous (red), anatase (green), and rutile (blue) phases for TiO_2-40, TiO_2-20, and TiO_2-10 samples calculated from the O K-edge by fitting reference spectra to the measured spectra (Figure S5 and S6) by least squares method. The left column shows the results of the bulk sensitive total yield measurements, and the right column shows the results of the more surface sensitive Auger yield measurements.

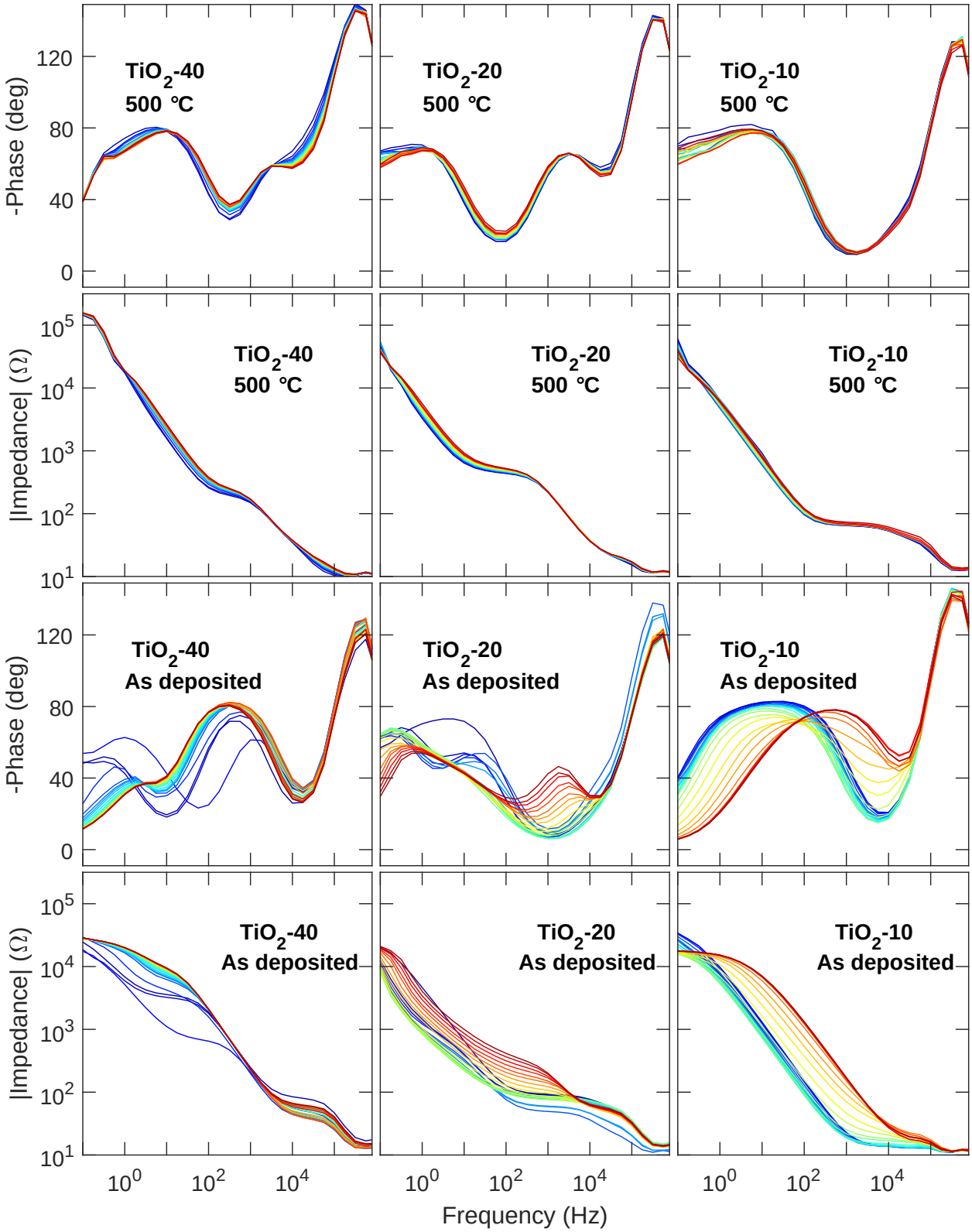

Fig. S8: The magnitude and phase of impedance measured with electrochemical impedance spectroscopy during stability tests in 1.0 M NaOH. For the as deposited samples the spectra are plotted from 1 h (blue) to 25 h (red) with 1 h increments, whereas for the 500 °C vacuum annealed samples the spectra are plotted from 4 h (blue) to 80 h (red) with 4 h increments.