

Experimentally informed structure optimization of amorphous TiO₂ films grown by atomic layer deposition

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XPS spectrums of free-standing TiO₂ film

Ti 2p core spectra was fitted with two peaks located at 458.4 eV and 464.2 eV corresponding to Ti 2p_{3/2} and Ti 2p_{1/2} with 5.8 eV peak separation which implied +4 valence for Ti. O 1s spectra showed the peak at 529.9 eV regarded as Ti-O bonds in TiO₂. Through the surface quantitative analysis on the integration of fitting peaks divided by the relative sensitive factor, the O/Ti ratio value was about 1.91, indicating stoichiometry TiO₂ with tiny oxygen vacancy.

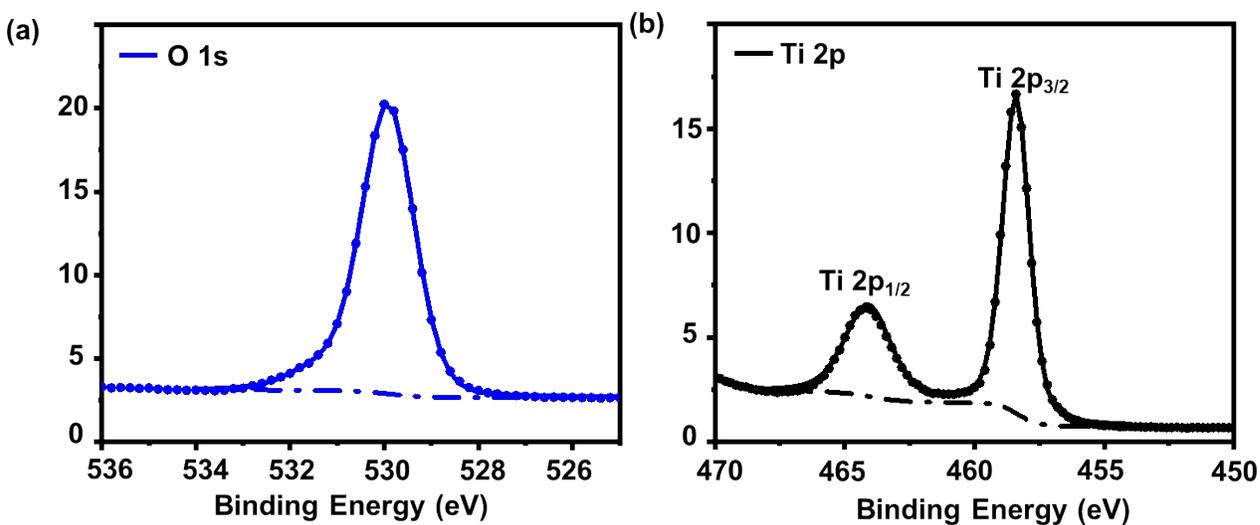


Figure S1. XPS spectrums of free-standing TiO₂ film grown under 100°C. a, O 1s core spectra. b, Ti 2p core spectra.

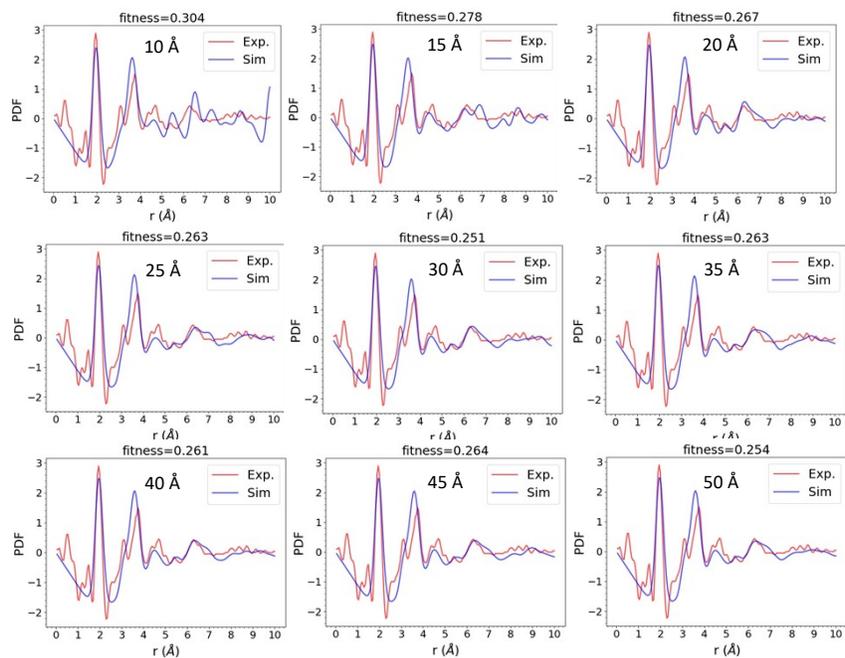


Figure S2. Simulated $G(r)$ of melt-quenched α - TiO_2 model with different size.

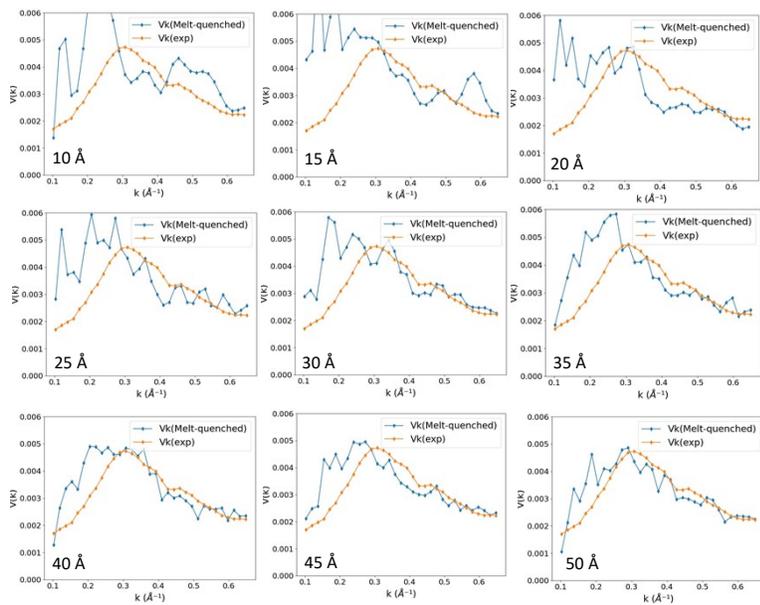


Figure S3. Simulated $V(k)$ of melt-quenched α - TiO_2 model with different size.