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Supplementary Information

Strain-boosted electrocatalytic activity for oxygen evolution in RuO_2 epitaxial thin films

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Experimental details

The RuO_2 thin films were grown on α-Al_2O_3 (0001) single crystal substrates by pulsed laser deposition. A RuO_2 pellet placed in a vacuum chamber with an O_2 partial pressure of 5 mTorr was irradiated by KrF excimer laser pulses (wavelength = 248 nm) with a fluence of 1.28 mJ cm^{-2} at a frequency of 10 Hz. The substrate temperature (T_s) was varied for thin films with an almost constant thickness of around 58 nm from 325 °C to 425 °C to control lattice strain. RuO_2 thin films with various thicknesses, ranging from 15 nm to 58 nm, were prepared at a constant T_s of 325 °C by adjusting the growth time (*i.e.*, the number of laser pulses) to investigate the thickness dependence of their electrochemical performance. X-ray diffraction patterns of the films were measured using a diffractometer (D8 DISCOVER, Bruker AXS) with Cu Kα radiation (wavelength = 1.5418 Å).

Electrochemical measurements were conducted on potentiostats (pocketSTAT, Ivium Technologies or Sp-200, Bio-Logic) using a standard three-electrode system, where a Pt wire and an Ag/AgCl electrode (saturated KCl) served as the counter and reference electrodes, respectively. 0.10 M KOH aqueous solution saturated with O_2 gas was used as the electrolyte. Linear sweep voltammetry was performed at a sweep rate of 10 mV sec^{-1}. The *iR* drop of potential was corrected using the series resistance determined by electrochemical impedance spectroscopy (Table S1, S2, and Fig. S1). The potential vs the reversible hydrogen electrode E_{RHE} was calculated from the following equation.

$$E_{RHE} = E_{AgCl} + 0.059\ pH + E^0_{AgCl}$$

where E_{AgCl} is the potential vs Ag/AgCl electrode (sat. KCl) and E^0_{AgCl} = 0.1976 eV at 298 K. Cyclic voltammetry was conducted in an aqueous solution of 0.10 M KOH, 5.0 mM $K_3[Fe(CN)_6]$, and 5.0 mM $K_4[Fe(CN)_6]$ saturated with Ar gas to investigate the influence of surface roughness.

Cross-sectional structural observations were performed by a 200 kV transmission electron microscope (JEM-ARM200F, JEOL). Thin film specimens were prepared by the focused ion beam method. High-angle annular dark-field and annular bright-field images were collected by scanning transmission electron microscope measurement for high-resolution observation.

X-ray fluorescence holography measurements were performed on RuO_2 thin films with *a*-axis strains of 0.8% and 4.4% at the beamline BL13XU of the synchrotron radiation facility

SPring-8, Japan. The Ru Kα fluorescent X-ray holograms were recorded with an avalanche photodiode detector at incident X-ray energies of 25.0–28.5 keV in 0.5 keV steps. Fig. S2 shows a representative hologram taken at 28.5 keV. Details of the experimental setup are described elsewhere.[S1] The atomic arrangements around Ru were reconstructed from the multiple-energy holograms using Barton's algorithm.[S2,S3]

Table S1. Fitting parameters for the fitting curves of the electrochemical impedance spectra shown in Fig. S1a.

T (°C)	R_S (Ω)	R_{CT} (Ω)	C (F)
325	420	5.79×10^3	2.29×10^{-5}
350	413	3.91×10^4	1.78×10^{-5}
375	422	5.79×10^4	1.67×10^{-5}
425	456	8.55×10^4	9.23×10^{-6}

Table S2. Fitting parameters for the fitting curves of the electrochemical impedance spectra shown in Fig. S1b.

t (nm)	R_S (Ω)	R_{CT} (Ω)	C (F)
15	500	7.67×10^3	1.85×10^{-5}
26	467	8.13×10^3	2.08×10^{-5}
58	420	5.79×10^3	2.29×10^{-5}

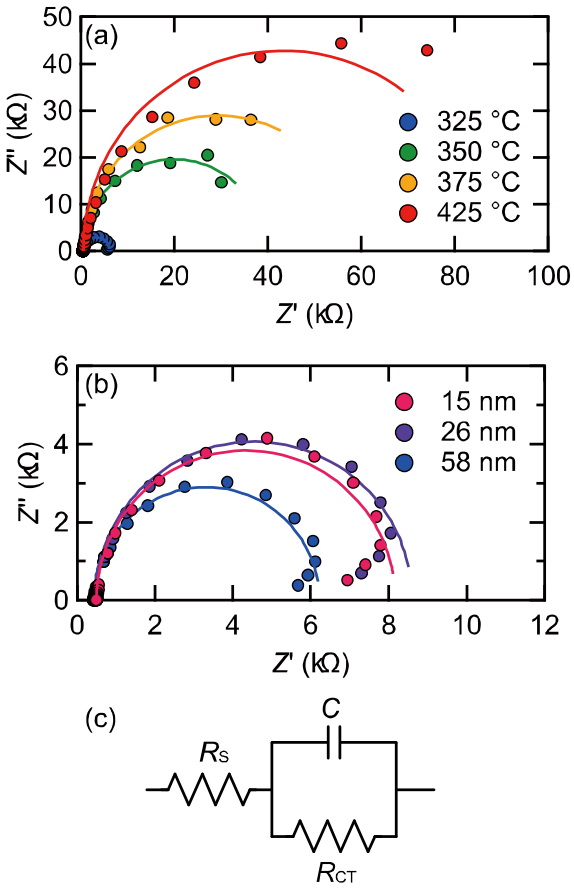

Fig. S1. (a,b) Electrochemical impedance spectra for RuO_2 epitaxial thin films grown (a) at various temperatures and (b) with various thicknesses. The curves show the results of fitting by the equivalent circuit shown in (c) where series resistance (R_s), capacitance (C), and charge transfer resistance (R_{CT}) are assumed.

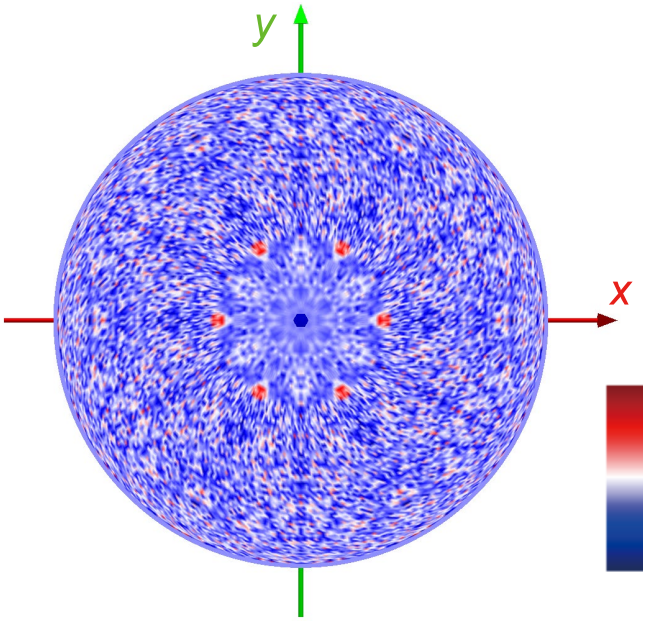

Figure S2. X-ray fluorescence hologram collected at 28.0 keV for RuO_2 epitaxial thin film with *a*-axis strain of 4.4%

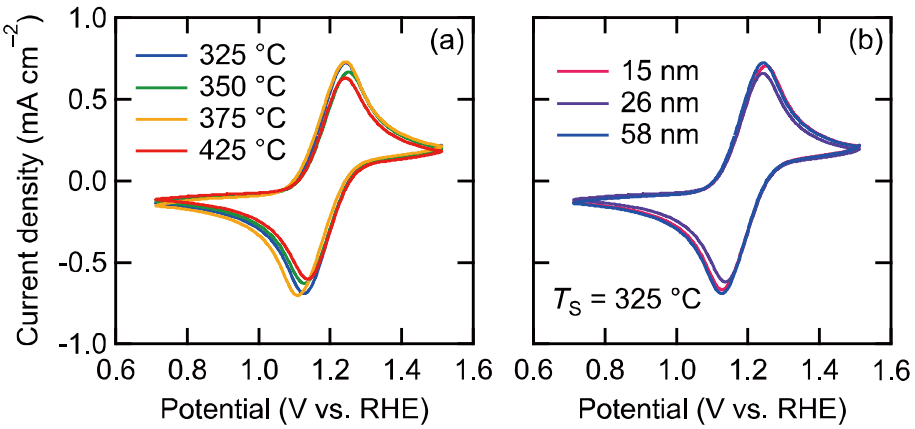

Figure S3. Cyclic voltammograms in $[Fe(CN)_6]^{3-/4-}$ solution for RuO_2 epitaxial thin films grown (a) at various temperatures and (b) with various thicknesses.

References

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