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# Supporting Information

**Thermal Atomic Layer Deposition of $Er_2O_3$ Films from a Volatile, Thermally Stable Enaminolate Precursor**

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## X-ray crystallographic details

The crystal structure of **1** was collected on a Bruker D8 Venture diffractometer with kappa geometry, an Incoatec IμS micro-focus X-ray source (Mo $K_\alpha$ radiation), and a multilayer mirror for monochromatization. The diffraction intensities were measured using a Bruker Photon III CPAD area detector. Data were acquired at 102 K with an Oxford 800 Cryostream low-temperature apparatus. The data were processed using APEX4 software. The structures were solved by Intrinsic Phasing using ShelXT and refined with ShelXL using Olex2. Hydrogen atoms were placed in calculated positions using a standard riding model and refined isotropically; all other atoms were refined anisotropically. The main refinement parameters are listed in Table S1. The crystal structure data were deposited with the Cambridge Crystallographic Data Centre, with the deposition number 2266444.

**Table S1.** Crystal data and structure refinement for **1**.

| | |
|---|---|
| Identification code | CHW_CD_ErL13_2 |
| Empirical formula | $C_{24}H_{48}ErN_3O_3$ |
| Formula weight | 593.91 |
| Temperature/K | 102.00 |
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a/Å | 9.8012(7) |
| b/Å | 21.6980(15) |
| c/Å | 14.4627(11) |
| α/° | 90 |
| β/° | 108.316(3) |
| γ/° | 90 |
| Volume/Å$^3$ | 2919.9(4) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.351 |
| μ/mm$^{-1}$ | 2.899 |
| F(000) | 1220.0 |
| Crystal size/mm$^3$ | 0.12 × 0.1 × 0.08 |
| Radiation | Mo Kα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.764 to 61.082 |
| Index ranges | -14 ≤ h ≤ 14, -31 ≤ k ≤ 31, -20 ≤ l ≤ 20 |
| Reflections collected | 128020 |
| Independent reflections | 8917 [$R_{int}$ = 0.0456, $R_{sigma}$ = 0.0173] |
| Data/restraints/parameters | 8917/0/295 |
| Goodness-of-fit on F$^2$ | 1.033 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0164, w$R_2$ = 0.0358 |
| Final R indexes [all data] | $R_1$ = 0.0190, w$R_2$ = 0.0366 |

**Table S2.** Bond Lengths for **1**.

| Atom | Atom | Length/Å | | Atom | Atom | Length/Å |
|---|---|---|---|---|---|---|
| Er1 | O3 | 2.1447(10) | | N2 | C9 | 1.4563(19) |
| Er1 | O2 | 2.1589(10) | | C18 | C19 | 1.5199(19) |
| Er1 | O1 | 2.1618(10) | | C18 | C17 | 1.332(2) |
| Er1 | N3 | 2.4980(12) | | C19 | C21 | 1.524(2) |
| Er1 | N1 | 2.5649(11) | | C19 | C20 | 1.531(2) |
| Er1 | N2 | 2.5066(12) | | C19 | C22 | 1.532(2) |
| O3 | C18 | 1.3284(17) | | C2 | C3 | 1.5194(19) |
| O2 | C10 | 1.3288(17) | | C2 | C1 | 1.3459(19) |
| O1 | C2 | 1.3347(16) | | C3 | C6 | 1.5280(19) |
| N3 | C17 | 1.4578(18) | | C3 | C5 | 1.533(2) |
| N3 | C23 | 1.477(2) | | C3 | C4 | 1.534(2) |
| N3 | C24 | 1.479(2) | | C10 | C9 | 1.342(2) |
| N1 | C8 | 1.4848(19) | | C10 | C11 | 1.522(2) |
| N1 | C7 | 1.4721(18) | | C11 | C12 | 1.531(2) |
| N1 | C1 | 1.4539(18) | | C11 | C13 | 1.523(2) |
| N2 | C15 | 1.479(2) | | C11 | C14 | 1.530(2) |
| N2 | C16 | 1.4780(19) | | | | |

**Table S3.** Bond Angles for **1**.

| Atom | Atom | Atom | Angle/˚ | | Atom | Atom | Atom | Angle/˚ |
|---|---|---|---|---|---|---|---|---|
| O3 | Er1 | O2 | 109.41(5) | | C9 | N2 | Er1 | 105.41(8) |
| O3 | Er1 | O1 | 103.88(4) | | C9 | N2 | C15 | 110.03(13) |
| O3 | Er1 | N3 | 72.16(4) | | C9 | N2 | C16 | 109.72(12) |
| O3 | Er1 | N1 | 160.45(4) | | O3 | C18 | C19 | 115.31(13) |
| O3 | Er1 | N2 | 86.65(4) | | O3 | C18 | C17 | 120.92(13) |
| O2 | Er1 | O1 | 143.00(4) | | C17 | C18 | C19 | 123.68(13) |
| O2 | Er1 | N3 | 97.67(4) | | C18 | C19 | C21 | 109.00(11) |
| O2 | Er1 | N1 | 83.52(4) | | C18 | C19 | C20 | 108.02(12) |
| O2 | Er1 | N2 | 72.01(4) | | C18 | C19 | C22 | 112.39(13) |
| O1 | Er1 | N3 | 107.64(4) | | C21 | C19 | C20 | 109.00(13) |
| O1 | Er1 | N1 | 69.33(4) | | C21 | C19 | C22 | 108.90(12) |
| O1 | Er1 | N2 | 94.68(4) | | C20 | C19 | C22 | 109.47(13) |
| N3 | Er1 | N1 | 92.05(4) | | C18 | C17 | N3 | 120.14(13) |
| N3 | Er1 | N2 | 152.12(4) | | O1 | C2 | C3 | 115.61(12) |
| N2 | Er1 | N1 | 111.76(4) | | O1 | C2 | C1 | 120.50(13) |
| C18 | O3 | Er1 | 121.47(9) | | C1 | C2 | C3 | 123.86(12) |
| C10 | O2 | Er1 | 121.25(9) | | C2 | C3 | C6 | 112.95(11) |
| C2 | O1 | Er1 | 121.80(9) | | C2 | C3 | C5 | 107.94(12) |
| C17 | N3 | Er1 | 105.28(8) | | C2 | C3 | C4 | 108.16(12) |
| C17 | N3 | C23 | 108.32(12) | | C6 | C3 | C5 | 108.69(12) |
| C17 | N3 | C24 | 109.72(12) | | C6 | C3 | C4 | 109.41(12) |
| C23 | N3 | Er1 | 112.54(9) | | C5 | C3 | C4 | 109.64(13) |
| C23 | N3 | C24 | 109.87(12) | | O2 | C10 | C9 | 120.98(13) |
| C24 | N3 | Er1 | 110.97(9) | | O2 | C10 | C11 | 114.89(13) |
| C8 | N1 | Er1 | 100.63(8) | | C9 | C10 | C11 | 124.12(13) |
| C7 | N1 | Er1 | 121.83(9) | | C2 | C1 | N1 | 117.90(12) |

| C7 | N1 | C8 | 107.87(11) | | C10 | C9 | N2 | 119.99(13) |
|---|---|---|---|---|---|---|---|---|
| C1 | N1 | Er1 | 104.97(8) | | C10 | C11 | C12 | 109.11(12) |
| C1 | N1 | C8 | 109.26(11) | | C10 | C11 | C13 | 108.27(14) |
| C1 | N1 | C7 | 111.40(12) | | C10 | C11 | C14 | 112.40(14) |
| C15 | N2 | Er1 | 113.40(9) | | C13 | C11 | C12 | 108.49(15) |
| C16 | N2 | Er1 | 110.38(9) | | C13 | C11 | C14 | 110.67(17) |
| C16 | N2 | C15 | 107.87(13) | | C14 | C11 | C12 | 107.83(15) |

**Table S4.** Thickness of an $Er_2O_3$ film deposited in a nanoscale trench with aspect ratio = 10. The thicknesses were measured at the locations indicated in Fig. S10.

| Position | Thickness (nm) |
|---|---|
| 1 | 11.02 |
| 2 | 10.2 |
| 3 | 15.9 |
| 4 | 10.01 |
| 5 | 14.12 |
| 6 | 11.01 |
| 7 | 13.03 |
| 8 | 10.21 |
| 9 | 10.58 |

**Figure S1.** ORTEP image of **1** with thermal ellipsoids at the 50% level. Hydrogen atoms were omitted for clarity.

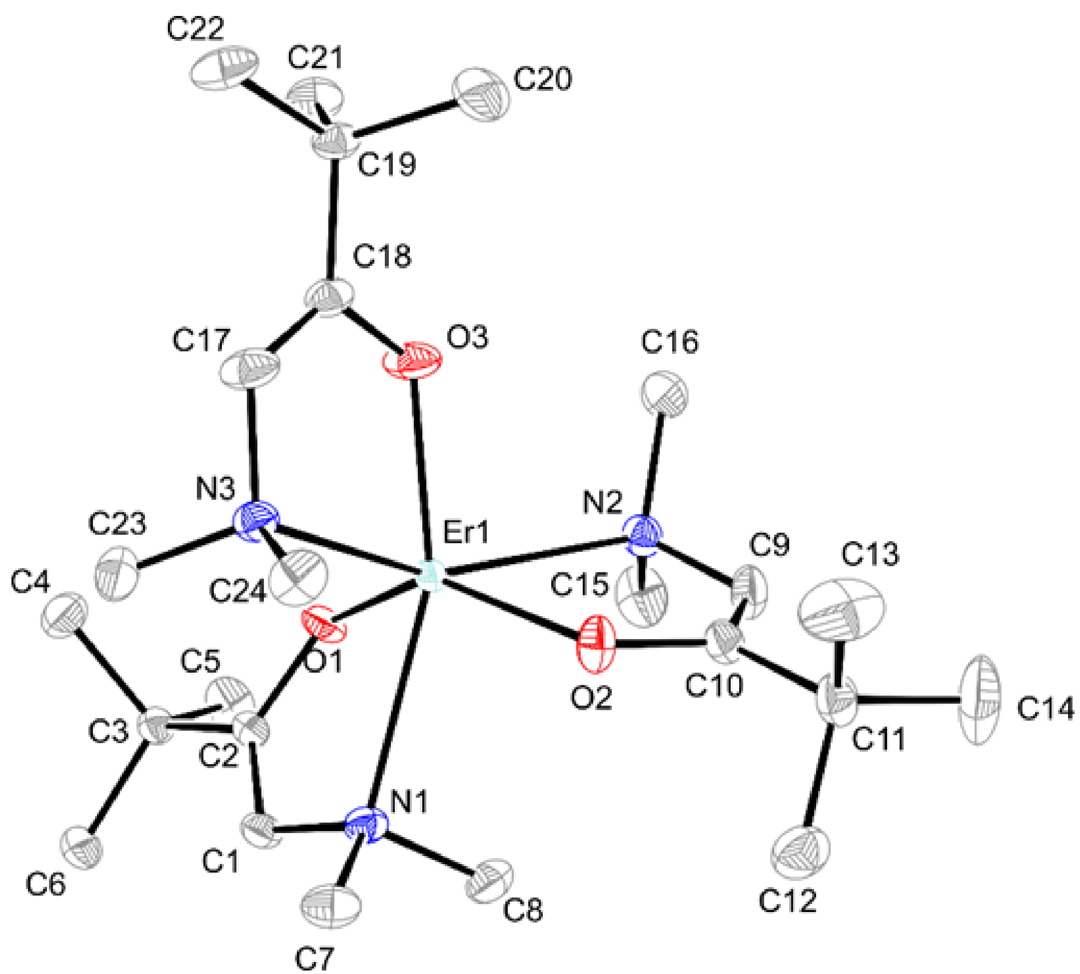


**Figure S2.** The dependence of $Er_2O_3$ film thicknesses on the number of ALD cycles on Si(100) substrates at 200 °C substrate temperature.

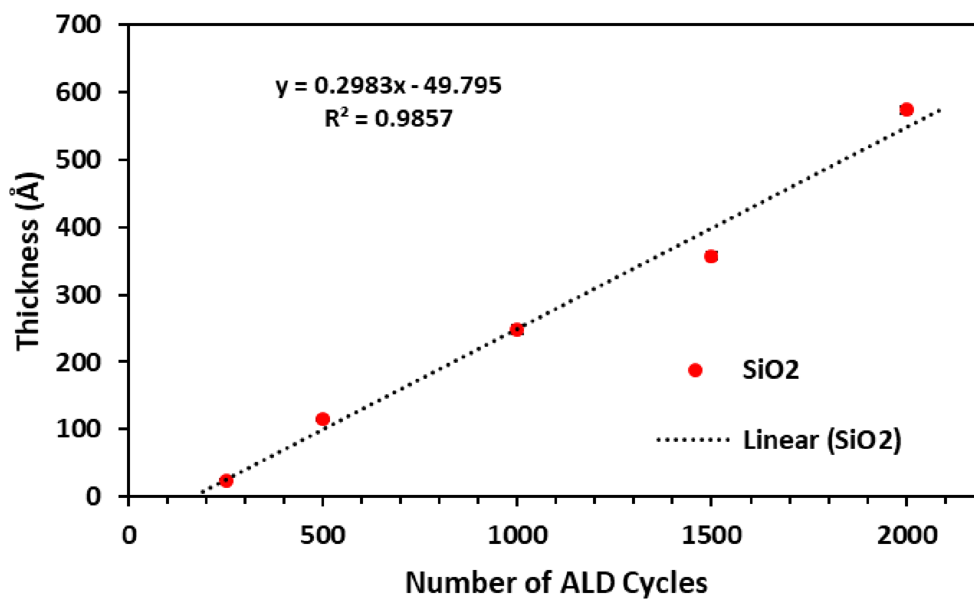


**Figure S3.** XRD patterns of ~20-25 nm as-deposited $Er_2O_3$ thin films deposited at 150, 200, and 250 °C on $SiO_2$ substrates with 1000 cycles. The dotted lines represent the reference for cubic $Er_2O_3$ (COD 1010334 $Er_2O_3$).

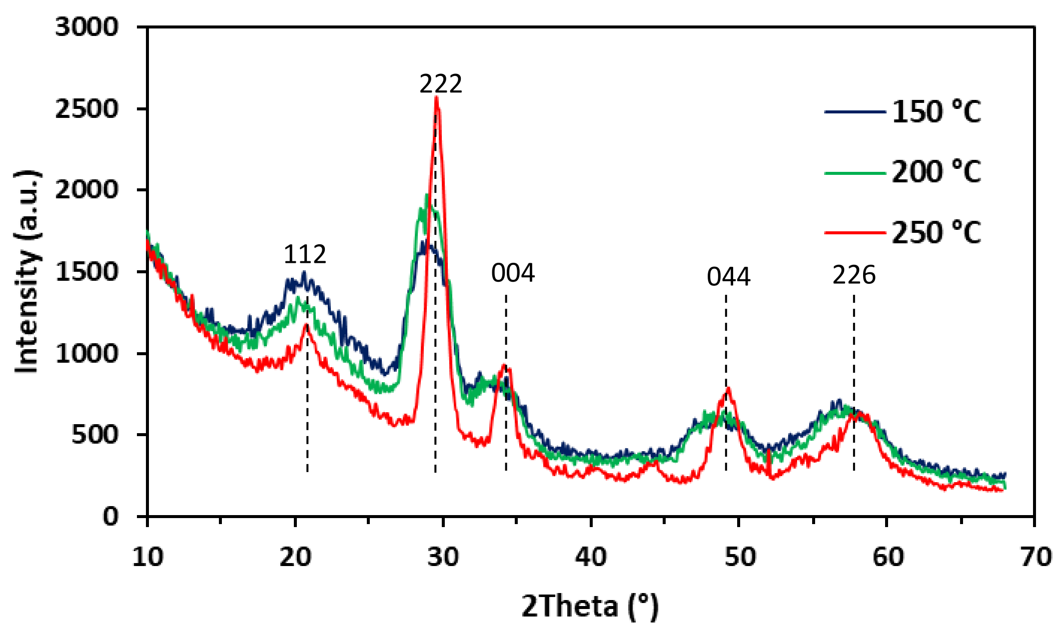
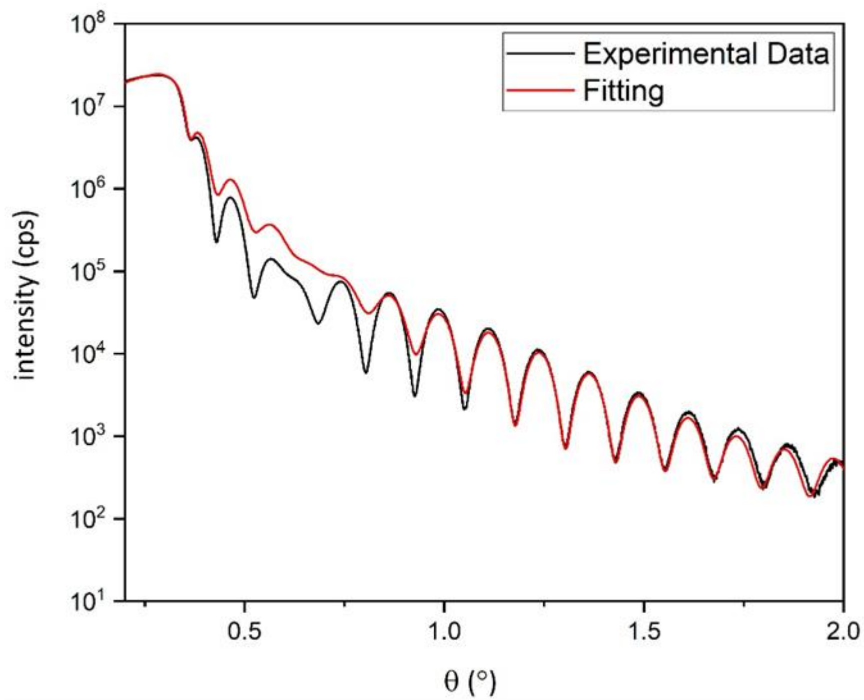


**Figure S4.** XRR fitting curves of 33 nm thick $Er_2O_3$ thin film grown on Si(100) (top, density = 7.3 gm/cm$^3$) and $SiO_2$ (bottom, density = 7.1 gm/cm$^3$) substrates at 200 °C.



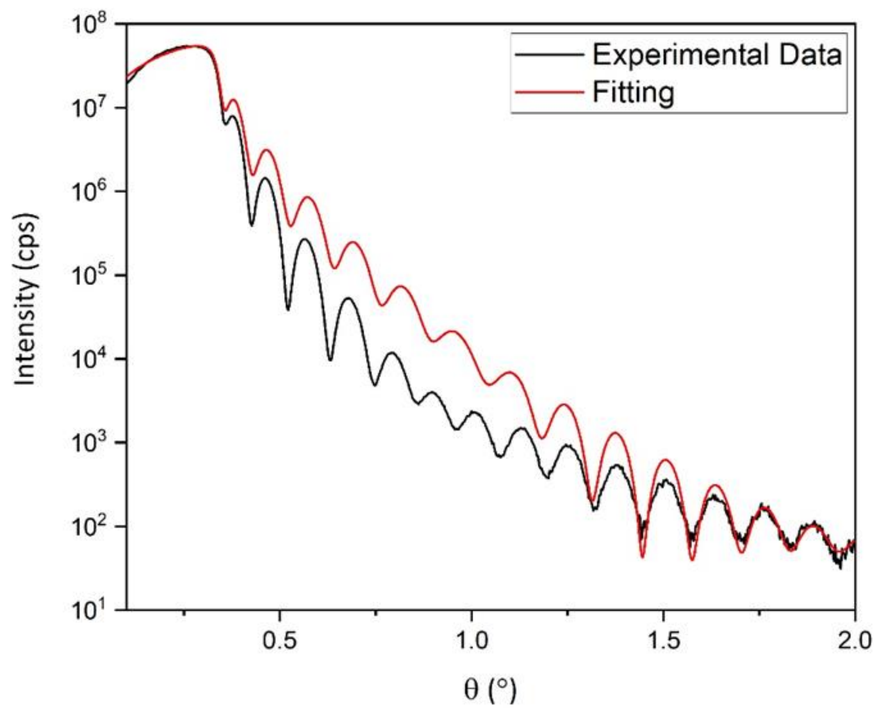
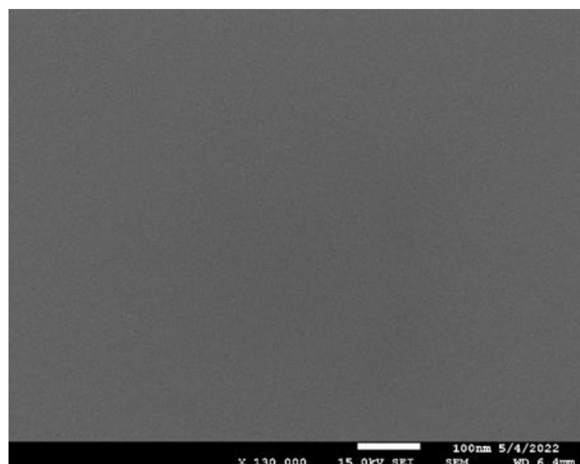



**Figure S5.** Top-down SEM micrographs of $Er_2O_3$ thin films deposited with 1500 ALD cycles on Si (left) and $SiO_2$ (right) substrates at 200 °C.



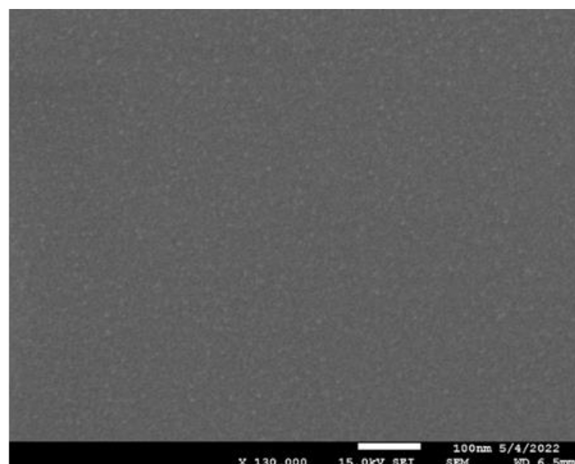



**Figure S6.** Cross-sectional SEM images of $Er_2O_3$ thin films grown on (a) Cu, (b) Ru, (c) TiN, (d) Pt, and (e) W at substrate temperatures of 200 °C with 1500 ALD cycles.

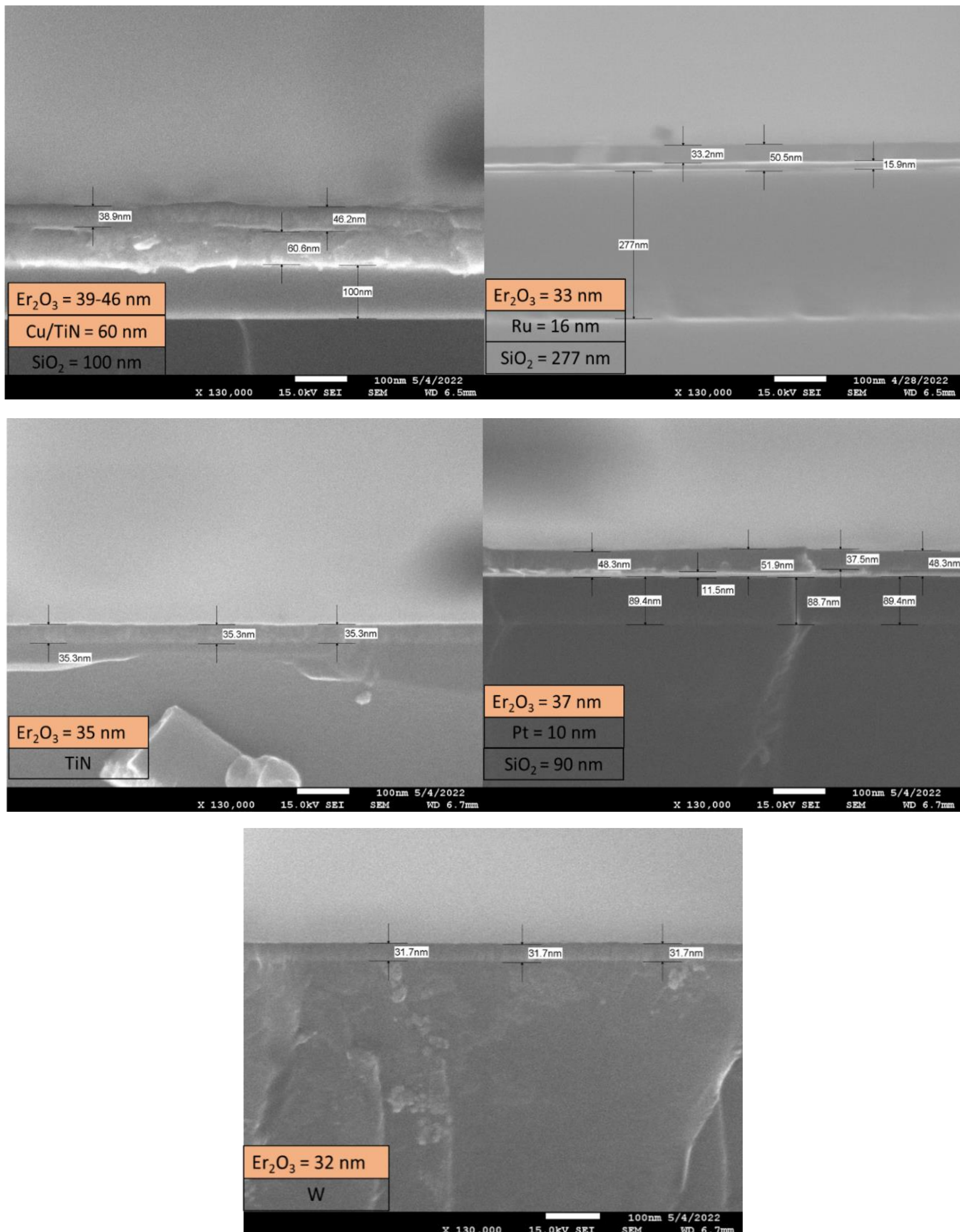


**Figure S7.** GI-XRD patterns of the as-deposited $Er_2O_3$ thin films shown in Fig. S6 grown on Cu, Ru, TiN, Pt, and W at substrate temperatures of 200 °C with 1500 ALD cycles.

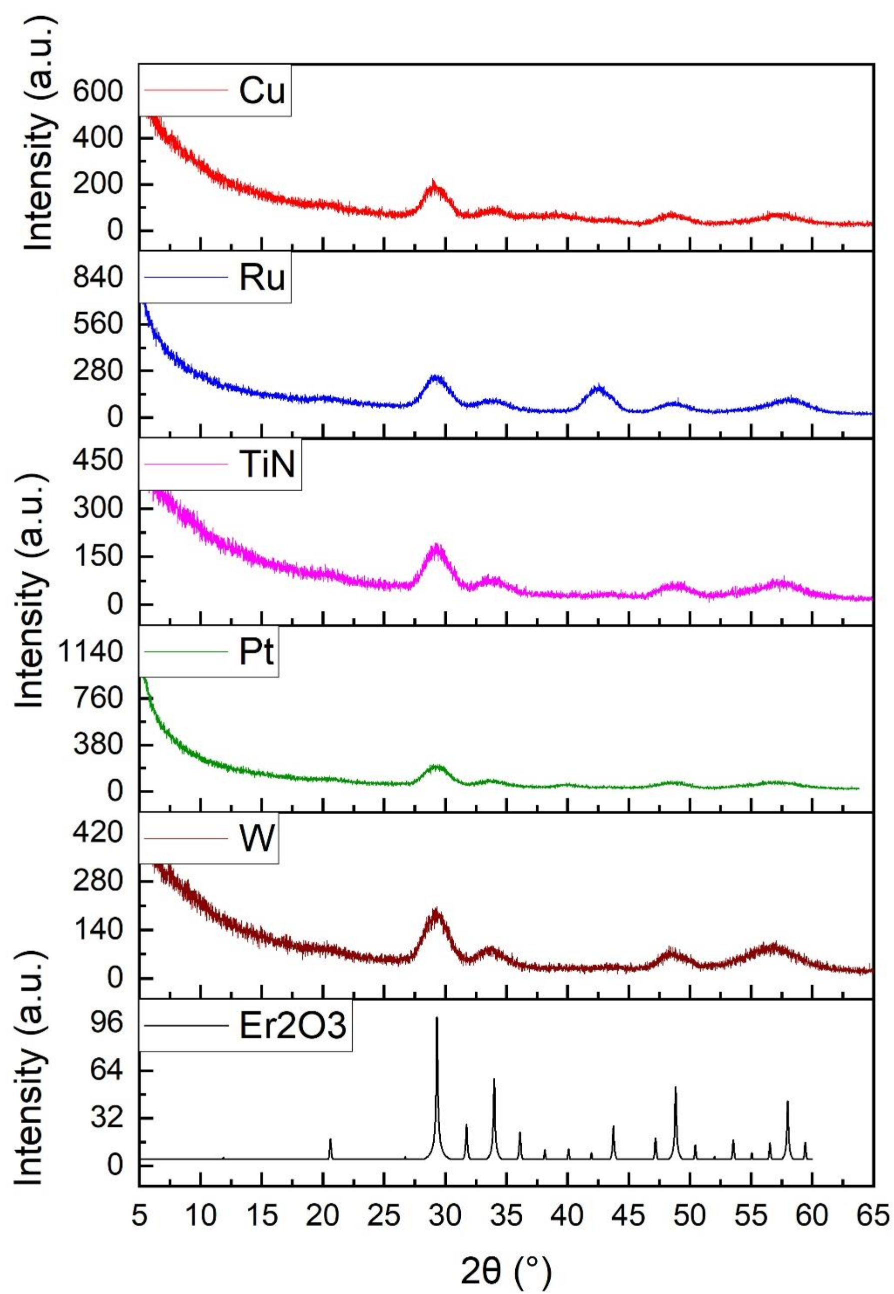


**Figure S8**. GI-XRD patterns of as-deposited $Er_2O_3$ thin films grown on an STO (top) and sapphire (bottom) at substrate temperatures of 200 °C with 1500 ALD cycles.

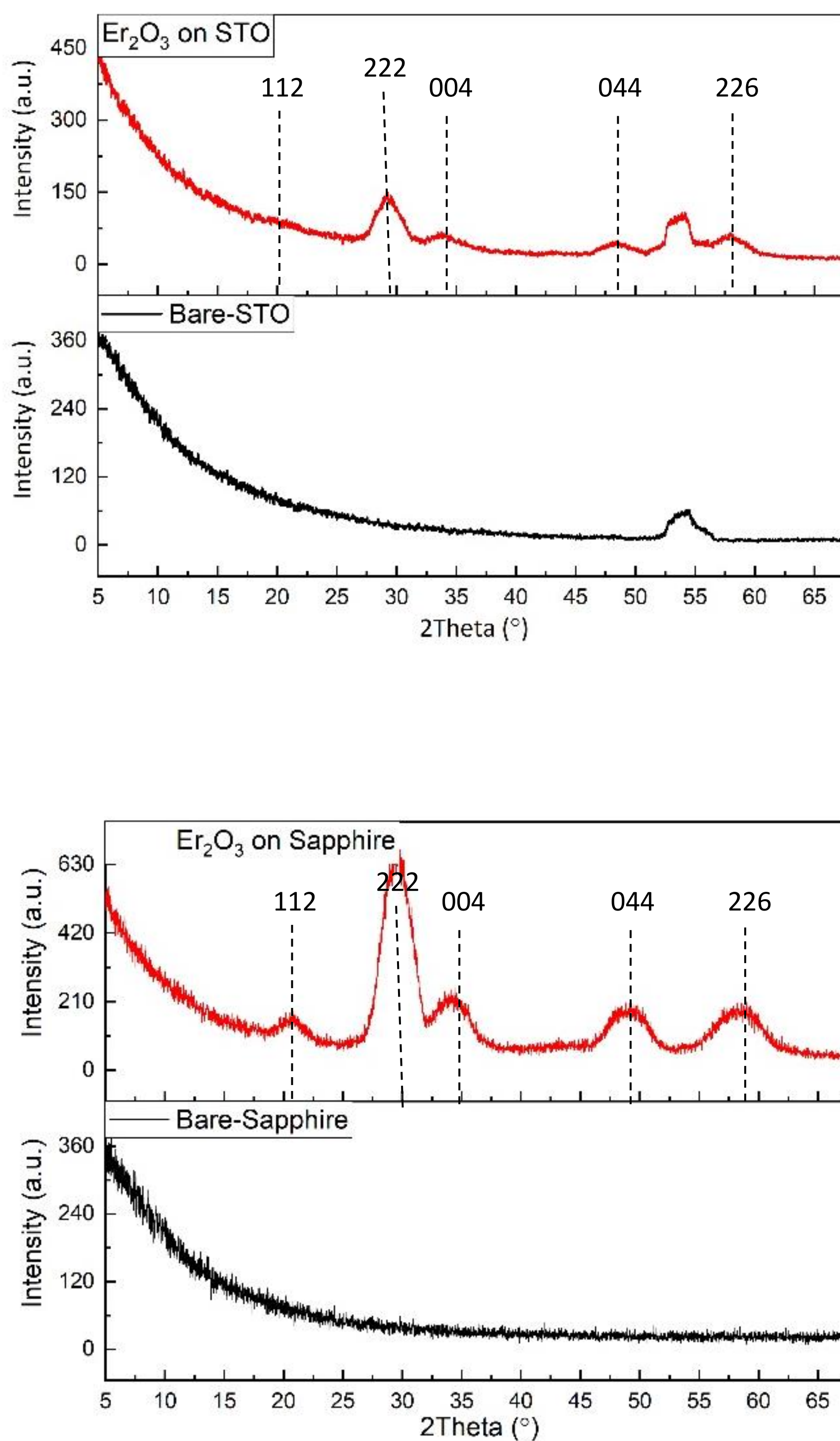
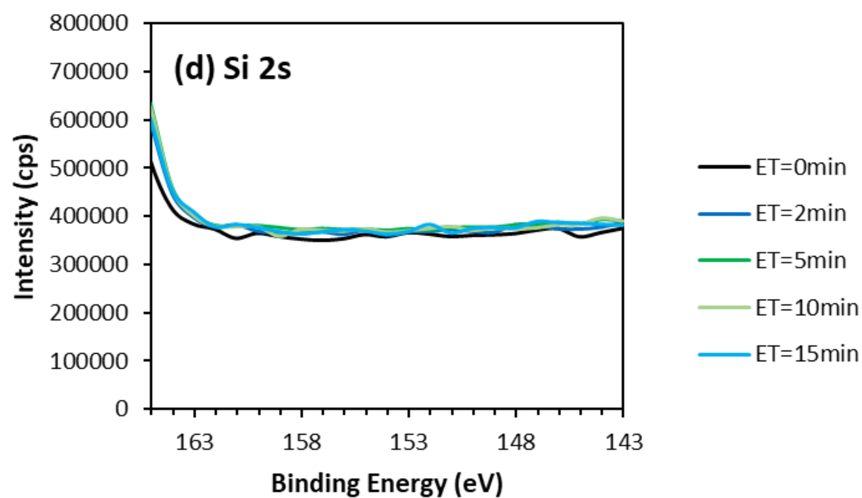
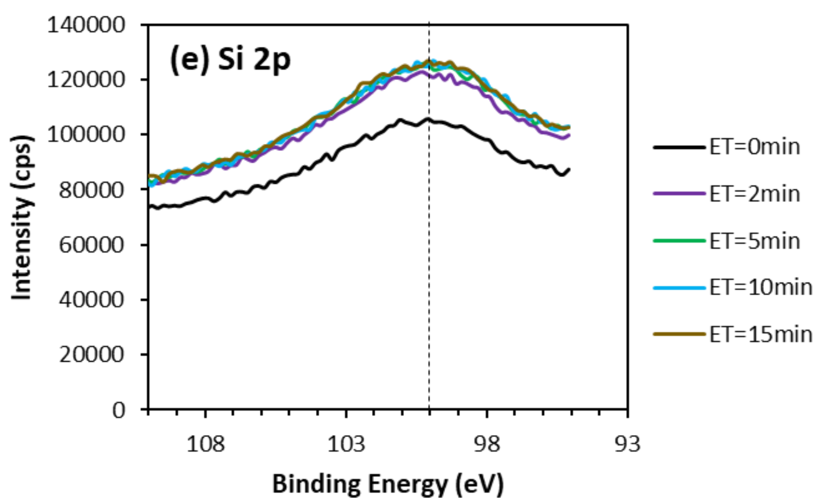
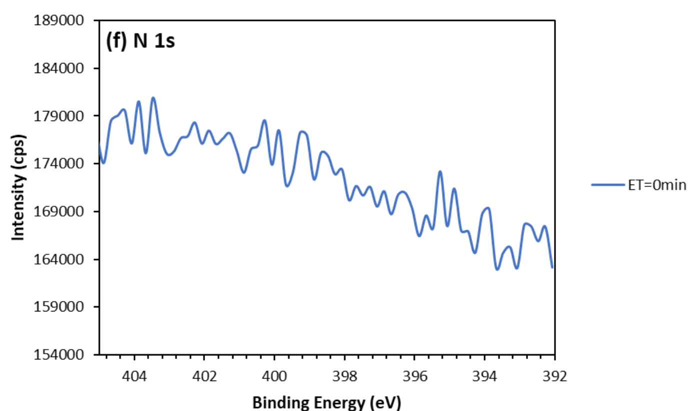


**Figure S9.** High-resolution XPS spectra of Si2s (d), Si2p (e), and N1s (f) ionization regions of a 35 nm thick $Er_2O_3$ thin film grown on Si(100) at a substrate temperature of 200 °C with 1500 cycles. These plots are a continuation of Fig. 7 in the text, and are numbered (d)-(g) to be compatible with Fig. 7.



(g) C 1s

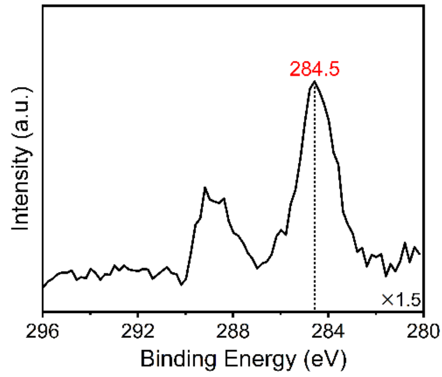



**Figure S10.** Er4d (a) and O1s (b) binding energy scans in the bulk of the film (after Ar ion sputtering), with peak fitting.

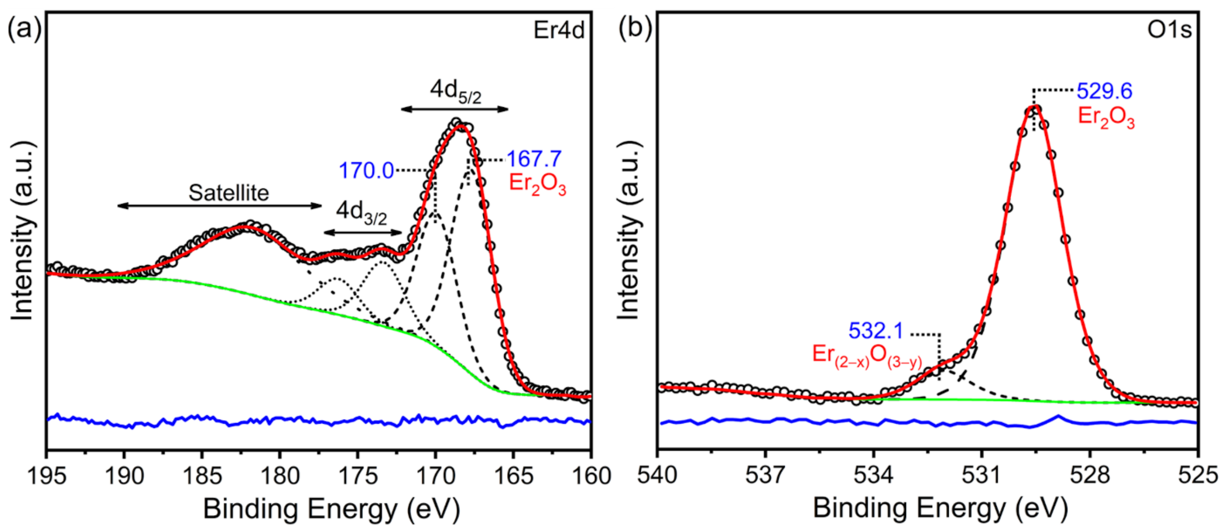



**Figure S11.** Overlapped EDS map of Er and Si elements. The numbered areas indicate the locations for the thickness measurements in Table S4.