**Cover Sheet**

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Fabrication of Ultra-Low Absorption Thin Films via Ion Beam Assisted Electron Beam Evaporation

Total Number of Page: 7

|  |  |
| --- | --- |
| List | Page |
| Authors | S1 |
| Manuscript Title | S1 |
| Table S1 | S4 |
| Table S2 | S4 |
| Figure S1 | S5 |
| Figure S2  Figure S3 | S6  S7 |

**Supporting Information:**

**Fabrication of Ultra-Low Absorption Thin Films via Ion Beam Assisted Electron Beam Evaporation**

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**Section 1. Bandgap data of all samples before and after annealing.**

All samples were annealed at 500°C, and their bandgap were calculated from the transmittance spectra using the Tauc equation. (Table S1)

The mass ratio of Ta2O5 to TiO2, denoted as m(Ta2O5/TiO2), represents the expected ratio during the coating process. Sample A consists of Ta2O5, sample B has 5%TiO2, sample C has 10%TiO2, sample D has 15%TiO2, sample E has 20%TiO2, and sample F consists of TiO2.

**Section 2. Normalized Raman spectrum of samples containing Ta2O5.**

The primary composition of samples A to E is tantalum oxide, and they exhibit similar spectral bands in the range of 550–750 cm⁻1, which are predominantly attributed to contributions from the thin film material. To provide a clearer visualization of the effects of doping and annealing on the Raman spectral bands of the thin films, this region was normalized, as shown in Figure S1.

**Section 3. The XPS spectra and peak fitting results of the thin films.**

The Ta, Ti, and O elements in the thin films were characterized through X-ray photoelectron spectroscopy (XPS) analysis. Figure 4 shows the XPS spectra of the films before annealing, while Figure S2 presents the XPS spectra after annealing. The peak fitting results for Ta4f7/2 are shown in Table 2, and the peak fitting results for Ti2p3/2 and O are provided in Table S2.

**Section 4. Relaxation structure of doping calculation model**

Doping was performed based on the Ta2O5 model obtained from molecular dynamics simulations. The results following structural relaxation after doping are presented in Figure S3.

**Table S1. Optical band gaps of the films before and after annealing.**

|  |  |  |
| --- | --- | --- |
| Sample ID | Optical bandgap(eV) |  |
|  | As deposited | Annealed |
| A | 4.169 | 4.199 |
| B | 3.953 | 4.034 |
| C | 3.574 | 3.634 |
| D | 3.504 | 3.554 |
| E | 3.415 | 3.478 |
| F | 3.246 | 3.268 |

**Table S2. Fitting results of Ti2p3/2 and O peaks in the films.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Sample | Ti2p3/2 | | O | |
| ID | As deposited | Annealing | As deposited | Annealing |
| A | -- | -- | 529.92 | 529.90 |
| B | 458.18 | 458.17 | 529.95 | 530.02 |
| C | 458.18 | 458.21 | 529.86 | 529.93 |
| D | 458.21 | 458.18 | 529.85 | 529.95 |
| E | 458.28 | 458.18 | 529.84 | 530.00 |
| F | 458.27 | 458.63 | 529.68 | 529.79 |



**Figure S1. Normalized Raman spectra of Ti-doped Ta2O5 thin films in the range of 550-750 cm-1.**



**Figure S2.** **Typical XPS spectra of annealed films: (a)** Ta 4f; **(b)** O 1s (OI refers to lattice oxygen, OII corresponds to hydroxyl groups, and OIII represents surface-adsorbed oxygen.); **(c)** Ti 2p.

**Figure S3. Computational model after structural relaxation: (a)** Ta2O5; **(b)** 1*VO*+1*TiTa*; **(c)** 1*VO*+2*TiTa*; **(d)** 1*VO*+3*TiTa*. *VO* represents an oxygen vacancy, which involves the removal of an Oxygen atom. *TiTa* refers to titanium doping, where a titanium atom replaces a tantalum atom. In the model, gold atoms represent Ta, red atoms represent O, and blue atoms represent Ti.