

Supporting Information

Entropy-Mediated Stable Structural Evolution of $(\text{HoErTmYbLu})_{0.2}\text{TaO}_4$ for High-Temperature Thermosensitive Applications

Jia Chen^{a,b}, Yafei Liu^{a,b}, Chaoyan Ma^a, Hao Sun^{a,b}, Yaxin Wei^a, Ruifeng Wu^{a,b}, Aimin Chang^a, Bo Zhang^{a*}

^aKey Laboratory of Functional Materials and Devices for Special Environmental Conditions (Chinese Academy of Sciences); Xinjiang Key Laboratory of Electronic Information Materials and Devices; Xinjiang Technical Institute of Physics & Chemistry of CAS, Urumqi 830011, China

^bCenter of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100049, China

*Corresponding author.

E-mail address:

zhangbocas@ms.xjb.ac.cn (Bo Zhang)

*E-mail address: zhangbocas@ms.xjb.ac.cn

*Present address: Xinjiang Technical Institute of Physics & Chemistry of CAS, Urumqi 830011, China

Table S1 Lattice parameters of RETaO₄ ceramics.

RETaO ₄	a	b	c	α	β	γ
HoTaO₄	5.3291	10.9329	5.0548	90	95.524	90
ErTaO₄	5.306	10.893	5.042	90	95.73	90
TmTaO₄	5.2769	5.438	5.0904	90	96.394	90
YbTaO₄	5.2508	5.4241	5.0678	90	96.171	90
LuTaO₄	5.238	5.425	5.057	90	96.04	90
(5RE)_{0.2}TaO	5.2655	5.4376	5.0806	90	96.272	90

Table S2 Comparison of this work and the latest research progress in high-temperature thermosensitive ceramics.

Samples	Temperature Range (°C)	Ageing Temperature (K)	B (K)	Aging coefficient after stabilization (%)
0.6MgAl₂O₄-0.4LaCr_{0.5}Mn_{0.5}O₃^[1]	573-273	1273	4163-8711	10
CeNbO₄^[2]	300-1523	1173	7547	19.73
(La_{0.2}Ce_{0.2}Nd_{0.2}Sm_{0.2}Eu_{0.2})NbO₄^[2]	300-1523	1173	4779	0.42
Ce_{1-2x}(NdSm)_x(VNbTa)_{1/3}O_{4+δ}^[3]	50-700	873	4600-6000	0.23-2.6
CeNbO₄-based^[4]	300-1623	1273	4697-5009	0.17-20
(HoErTmYbLu)_{0.2}TaO₄ (This work)	673-1773	1773	12851	3

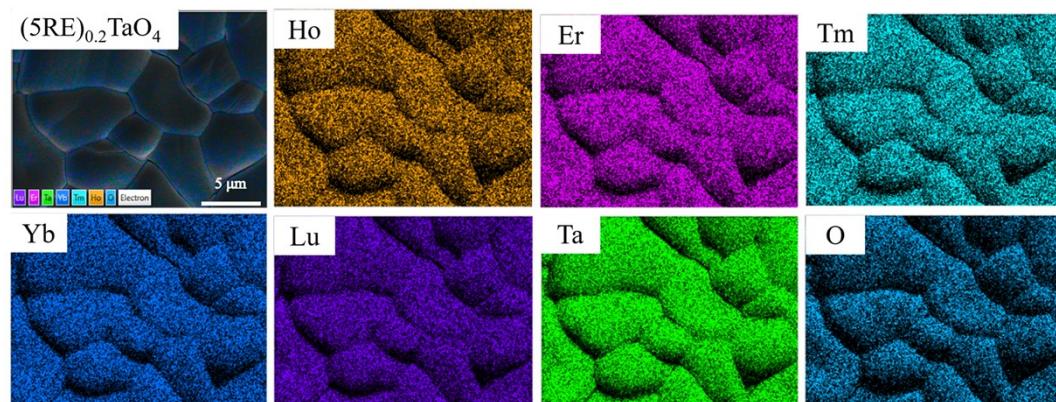


Fig. S1 Element distribution of (5RE)_{0.2}TaO₄.

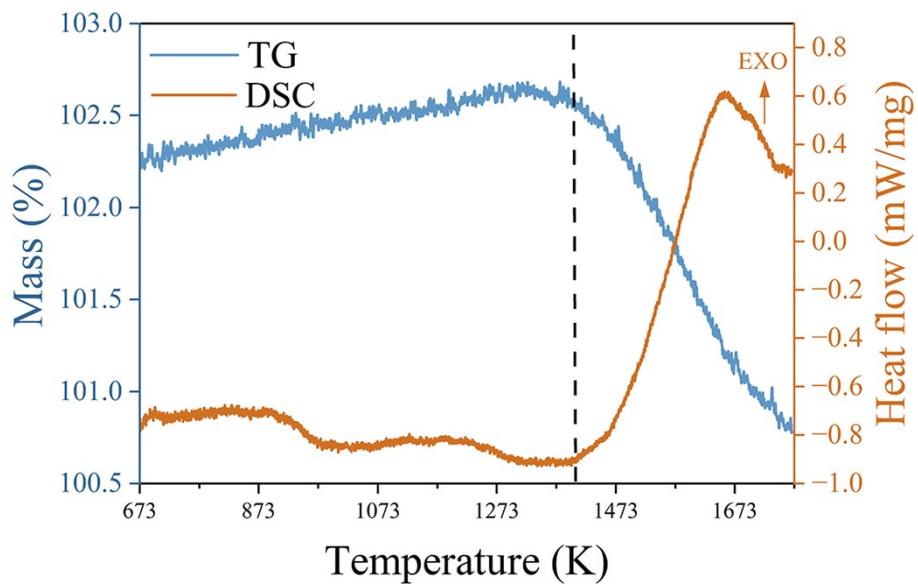


Fig. S2 TG-DSC curves of $(5\text{RE})_{0.2}\text{TaO}_4$ under an air atmosphere.

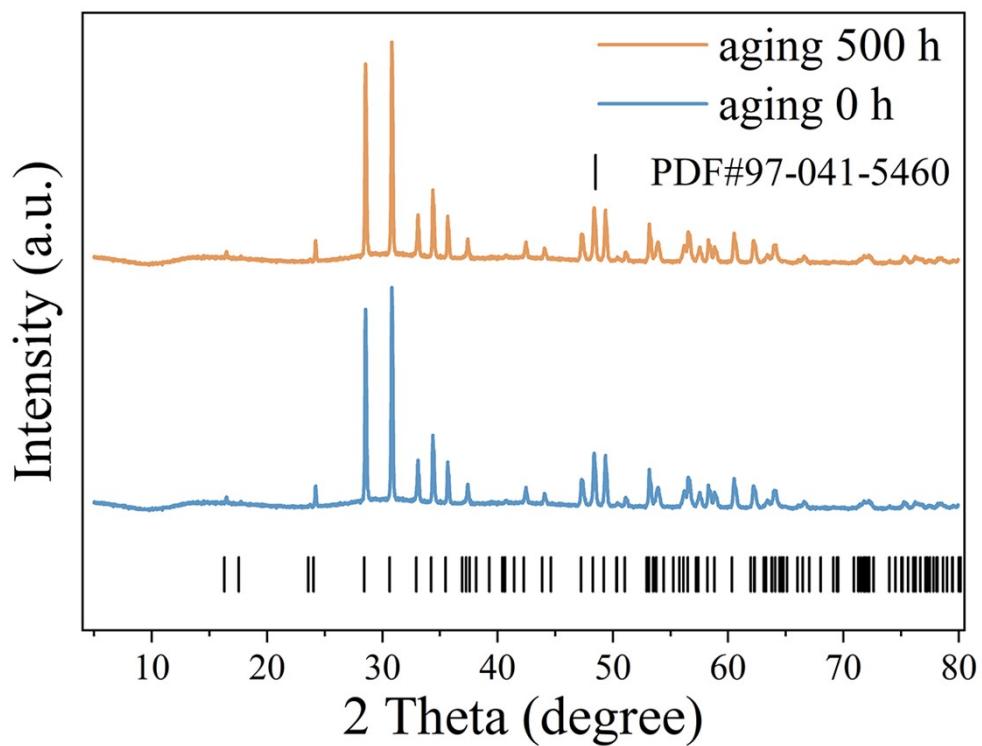


Fig. S3 XRD patterns of $(5\text{RE})_{0.2}\text{TaO}_4$ before and after aging.

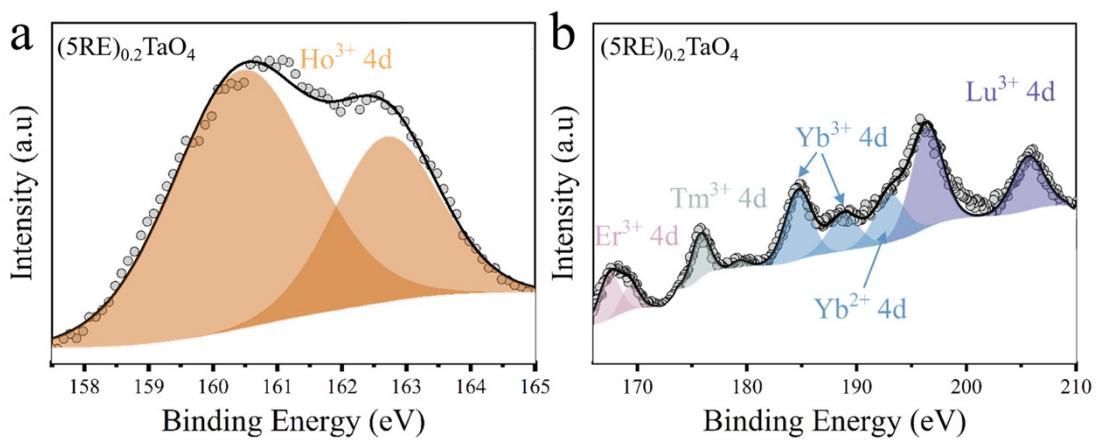


Fig. S4 XPS spectra of the $(5\text{RE})_{0.2}\text{TaO}_4$. (a) Ho 4d XPS spectra. (b) Er 4d, Tm 4d, Yb 4d and Lu 4d XPS spectra.

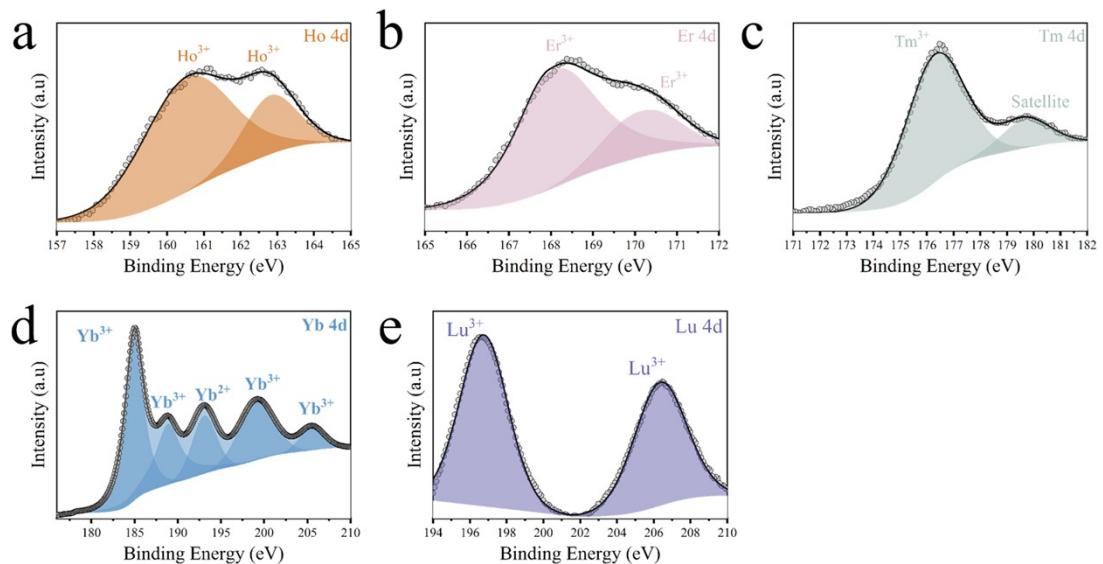


Fig. S5 XPS spectra of all samples except the $(5\text{RE})_{0.2}\text{TaO}_4$. (a) Ho 4d XPS spectra of HoTaO₄. (b) Er 4d XPS spectra of ErTaO₄. (c) Tm 4d XPS spectra of TmTaO₄. (d) Yb 4d XPS spectra of YbTaO₄. (e) Lu 4d XPS spectra of LuTaO₄.

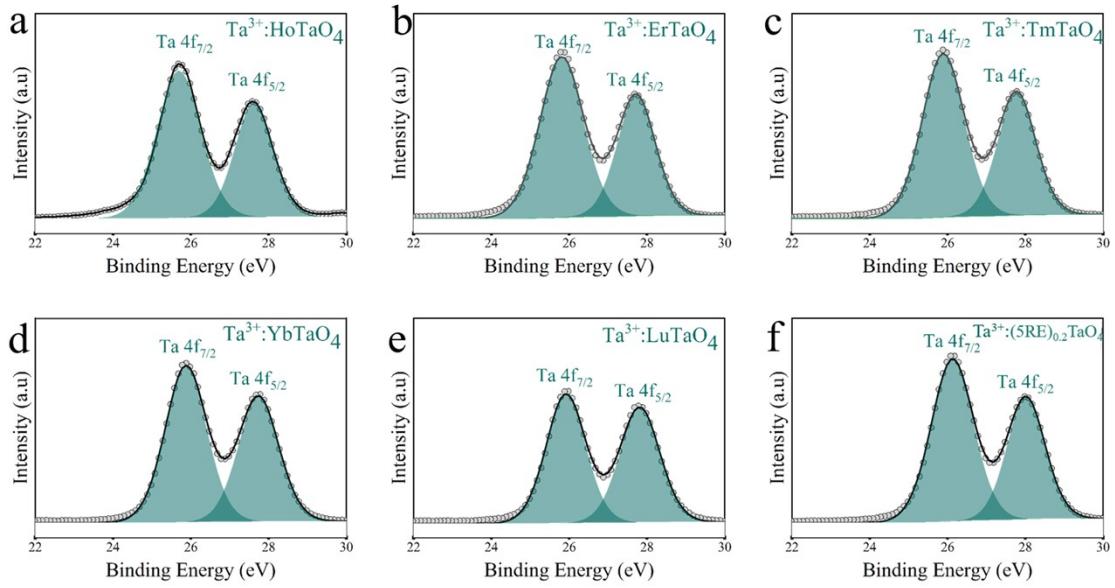


Fig. S6 Ta 4f XPS spectra of all samples. (a) Ta 4f XPS spectra of HoTaO₄. (b) Ta 4f XPS spectra of ErTaO₄. (c) Ta 4f XPS spectra of TmTaO₄. (d) Ta 4f XPS spectra of YbTaO₄. (e) Ta 4f XPS spectra of LuTaO₄. (f) Ta 4f XPS spectra of (5RE)_{0.2}TaO₄.

References

1. B. Zhang, Q. Zhao, H.X. Yan, Y.Q. Wu, *J. Mater. Sci.-Mater. Electron.*, 24 (2013) 4452–4456.
2. H. Sun, Y. Wang, Y. Liu, R. Wu, A. Chang, P. Zhao, B. Zhang, *ACS Appl. Mater. Interfaces.*, 16 (2024) 12821-12832.
3. Y. Liu, R. Wu, H. Sun, A. Chang, J. Guo, B. Zhang, *ACS Appl. Mater. Interfaces*, 16 (2024) 28861-28873.
4. Y. Liu, Y. Wei, R. Wu, Z. Fu, A. Chang, B. Zhang, *J. Eur. Ceram. Soc.*, 44 (2024) 311-318.