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Supplementary Material

Insights into roles of MgO additive in crystal structures, sintering behaviors, and optical properties of transparent In_2O_3 semiconductor ceramics

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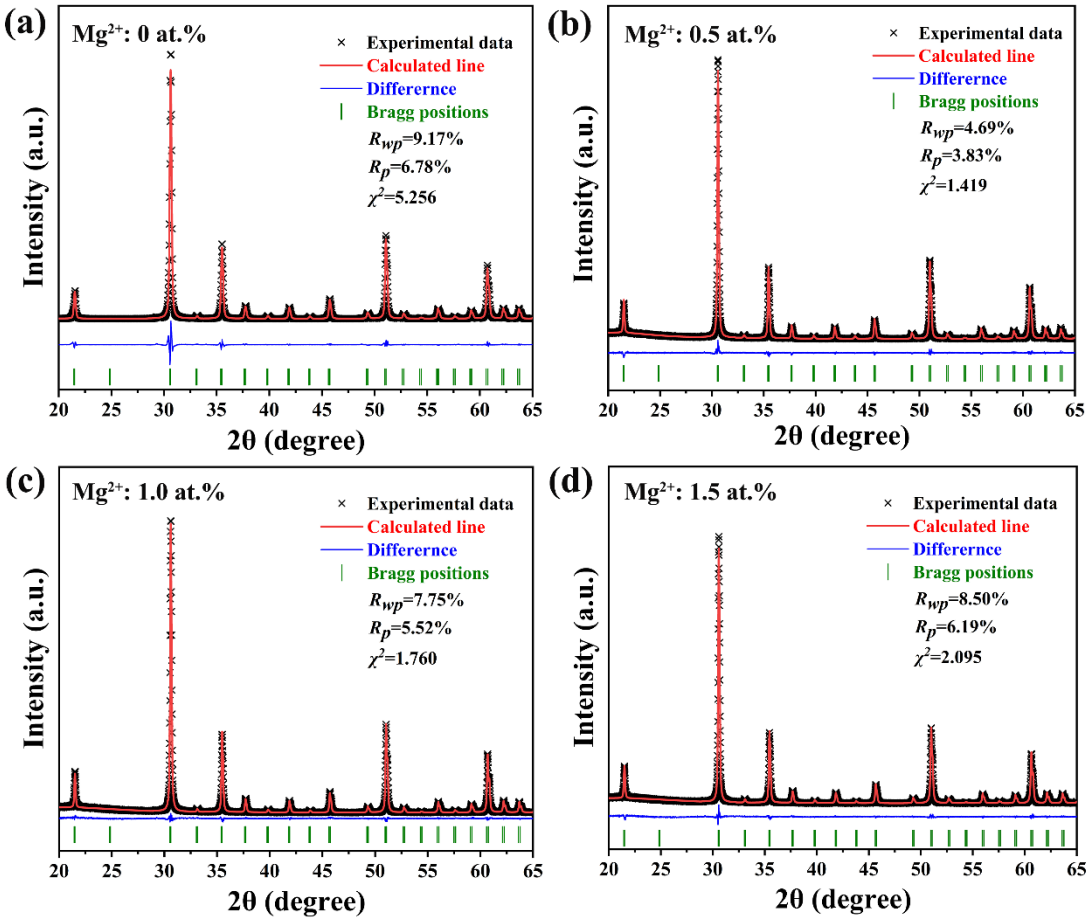

Fig. S1. XRD Rietveld refinement results for resulting In_2O_3 powders doped with 0 (a), 0.5 (b), 1.0 (c), and 1.5 (d) at.% MgO.

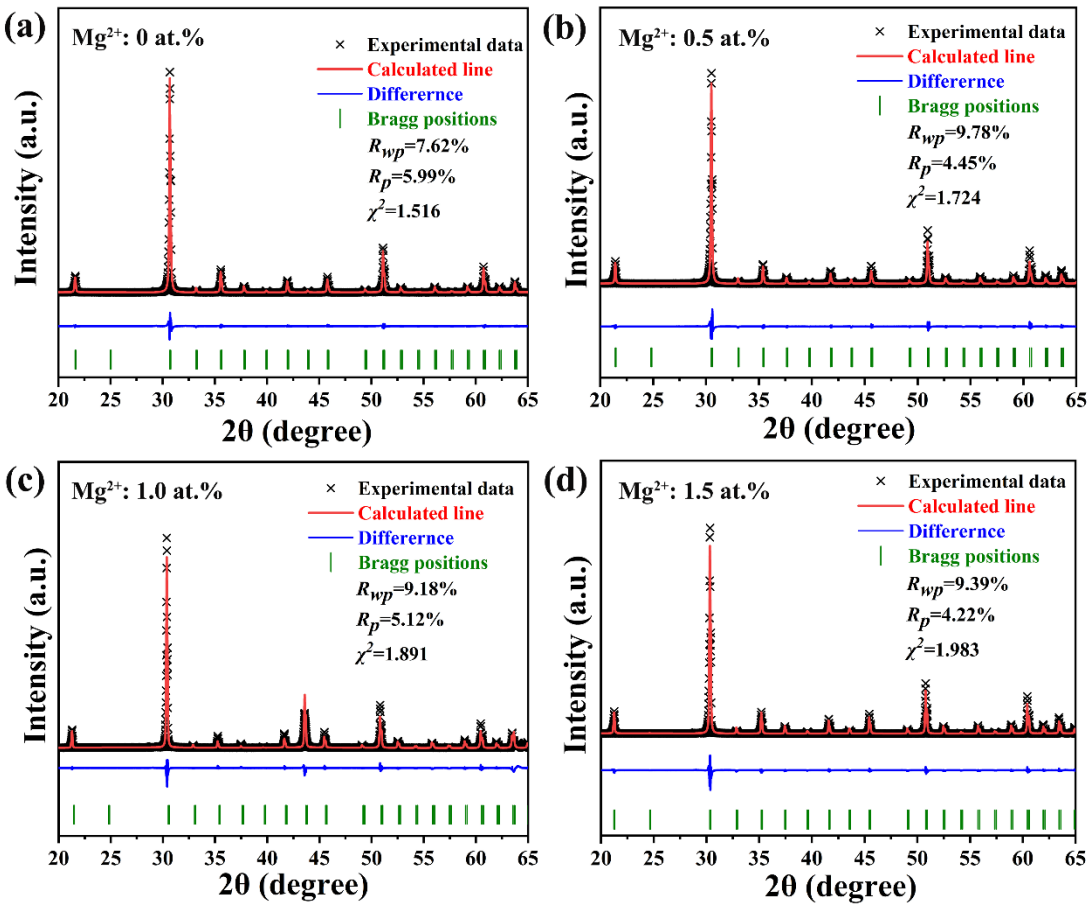

Fig. S2. XRD Rietveld refinement results for resulting In_2O_3 ceramics doped with 0 (a), 0.5 (b), 1.0 (c), and 1.5 (d) at.% MgO.

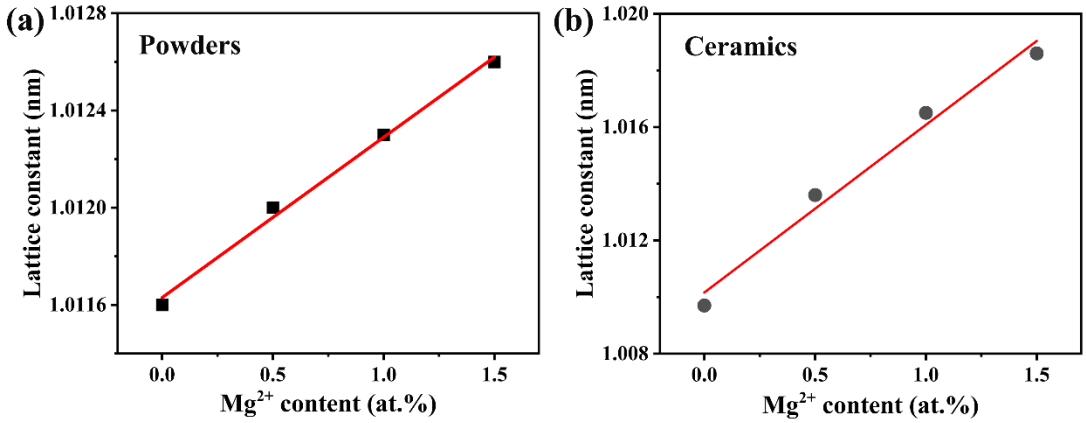

Fig. S3. Lattice constants of the In_2O_3 powders (a) and ceramics (b) as a function of Mg^{2+} content.

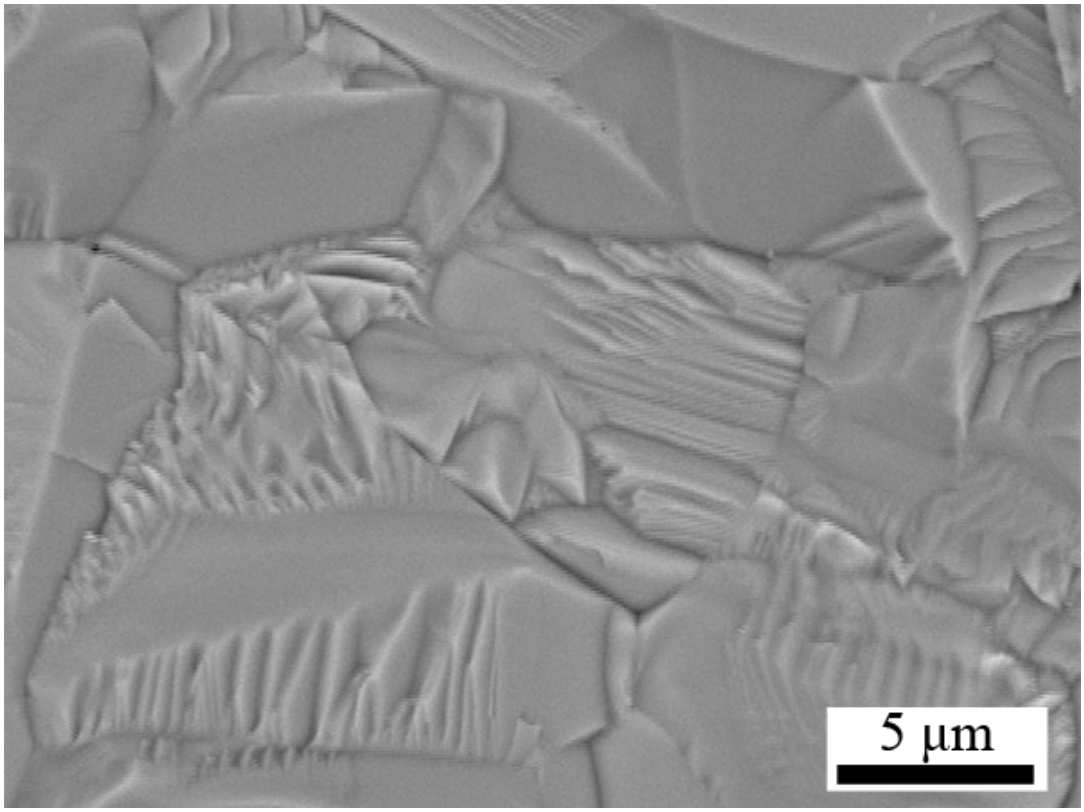

Fig. S4. Tabletop microscope micrograph showing the fracture surface of the 0.5 at.% Mg^{2+} doped In_2O_3 ceramic as representative.

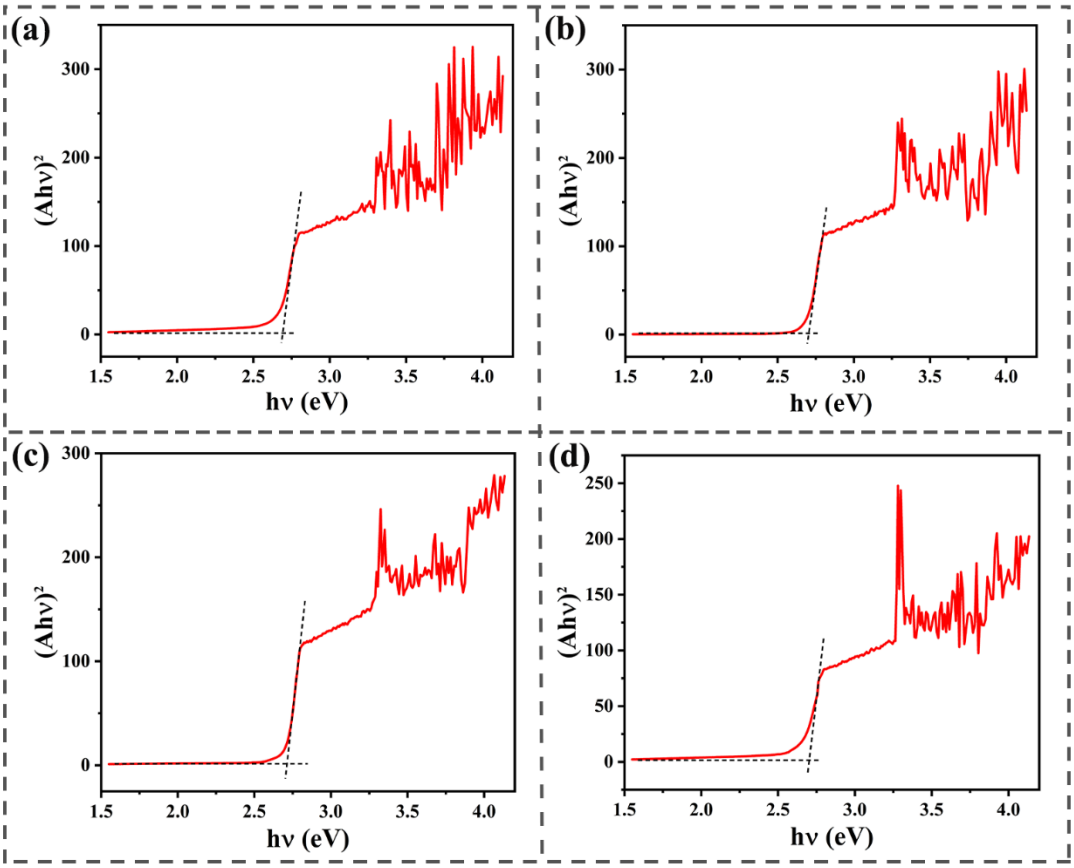

Fig. S5. A plots of $h\upsilon$ versus $(Ah\upsilon)^2$ obtained from the in-line transmittance curve of In_2O_3 ceramic samples with 0 (a), 0.5 (b), 1.0 (c) and 1.5 (d) at.% Mg^{2+} doping..

The previously reported direct bandgap energy of cubic In_2O_3 fell into the scope either 2.6−2.9 eV or 3.6−3.75 eV.[1-5] The experimental bandgap energy (E_g) of In_2O_3 bulks can be deduced from the transmittance cure based on Eqs. (1) and (2).

$$(\alpha h\upsilon)^2 = A(h\upsilon - E_g) \quad (1)$$

$$\alpha = \frac{1}{d}\ln(\frac{1}{T}) \quad (2)$$

where α is the absorption coefficient, $h\upsilon$ is the incident photon energy, A is the absorption constant, T is the transmittance, and d is the sample thickness. Therefore, a plot of $(Ah\upsilon)^2$ against $h\upsilon$ can estimate the E_g value by extrapolation of the linear part

of the curve to the *x*-axis ($y = 0$). This method results in a similar bandgap energy of ~2.7 eV for the four In_2O_3 bulk specimens with 0−1.5 at.% Mg^{2+} doping as shown in Fig. S5. Although this value is consistent with previous reports around 2.6−2.9 eV, the Tauc result may be affected by color center or light scattering.[6] That is, such a narrow bandgap is not enough to yield the near-UV emission as shown in Fig. 7(a) of the main text. Therefore, we believe that the reported bandgap energy of 3.6−3.75 eV is more acceptable.

References

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