

Supplemental Materials:
Reaction at buried Ti/ZnO thin film interface as seen by hard x-ray
photoemission and thermal desorption spectroscopy

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1. Complementary Figures

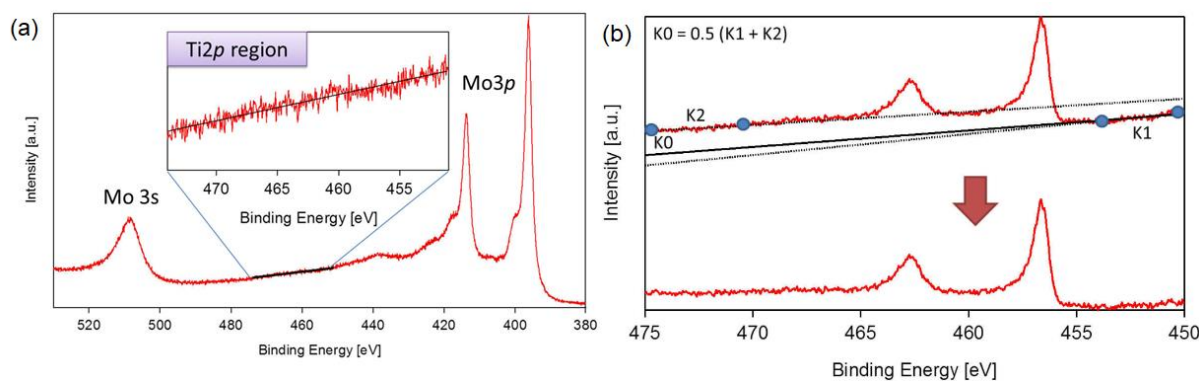


Fig. S1. (a) HAXPES spectrum of a Si_{wafer}/ZnO(29.7nm)/Mo(4.9nm) sample in the Ti 2p core level region showing the linear behavior of the Mo 3p inelastic background. (b) Example of the linear background subtraction methodology on the Si_{wafer}/ZnO(29.7nm)/Ti(3.6nm)/Mo(4.9nm) sample.

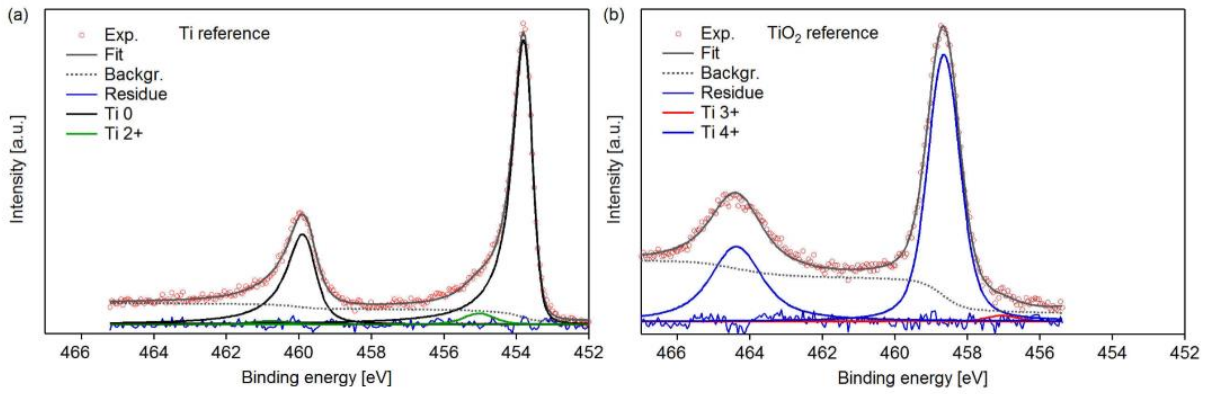


Fig. S2. Fit of Ti 2*p* core level of (a) Si_{waf}/Ti(44.1nm)/Mo(4.9nm) and (b) Si_{waf}/TiO₂(20nm)/Mo(5.0nm) reference stacks with mainly (a) metallic Ti⁰ and (b) fully oxidized Ti⁴⁺ components: (red circles): data, (black line): fit, (dotted line): background; (blue line): residue, (others) indicated oxidation states of Ti.

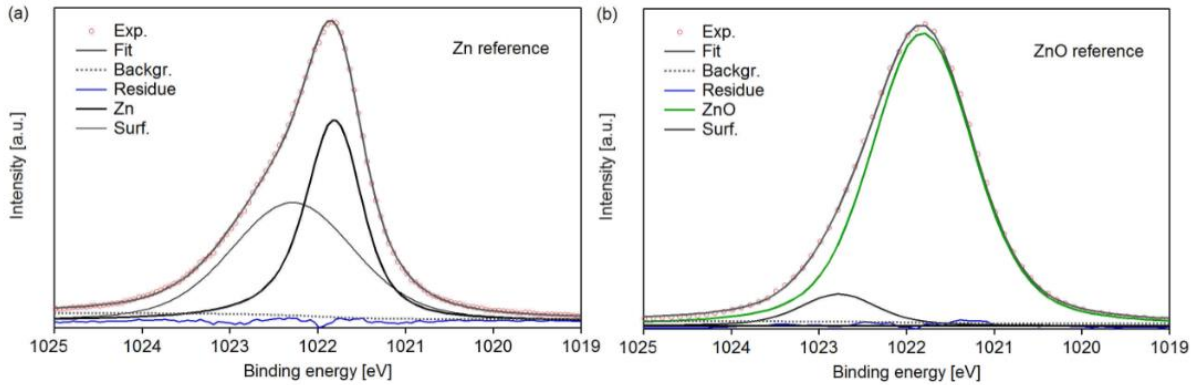


Fig. S3. Fit of Zn 2*p* core level of (a) Si_{waf}/Zn(15nm) and (b) Si_{waf}/ZnO(29.9nm)@RT reference stacks. The unfortunate lack of capping leads to a surface contamination peak (oxidized Zn and/or hydroxydes): (red circles): data, (black line): fit, (dotted line): background; (blue line): residue, (others) bulk and surface peaks.

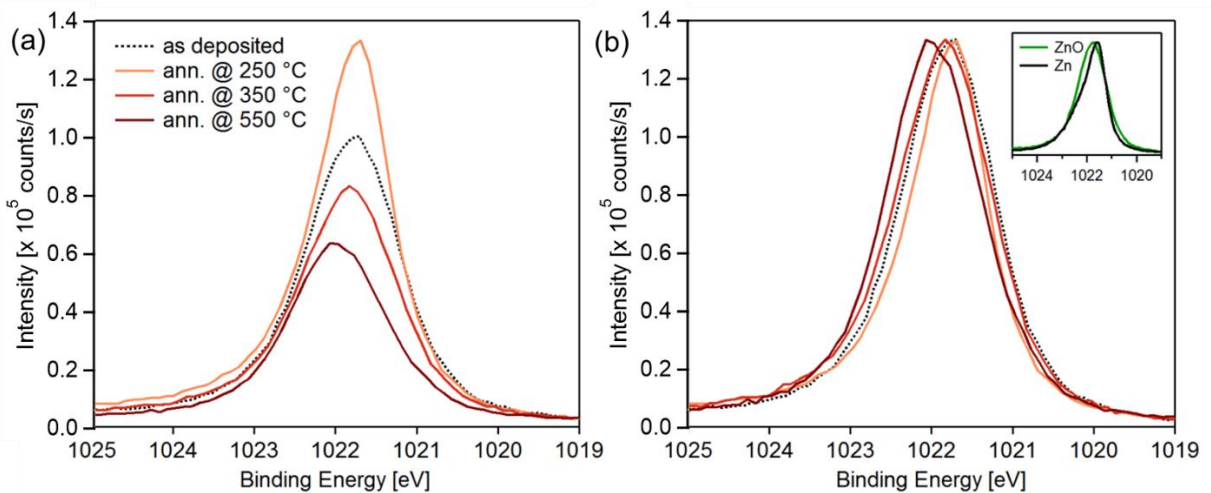


Fig. S4. Evolution of Zn 2*p* 3/2 core level of the 29.7@RT stack (Si_{waf}/ZnO(29.7nm)/Ti(3.5nm)/Mo(5nm)): upon annealing on (a) an absolute scale of intensity and (b) after normalization to the peak

maximum. The inset shows the profiles of Zn 2p 3/2 for the above discussed metallic Zn and ZnO references.

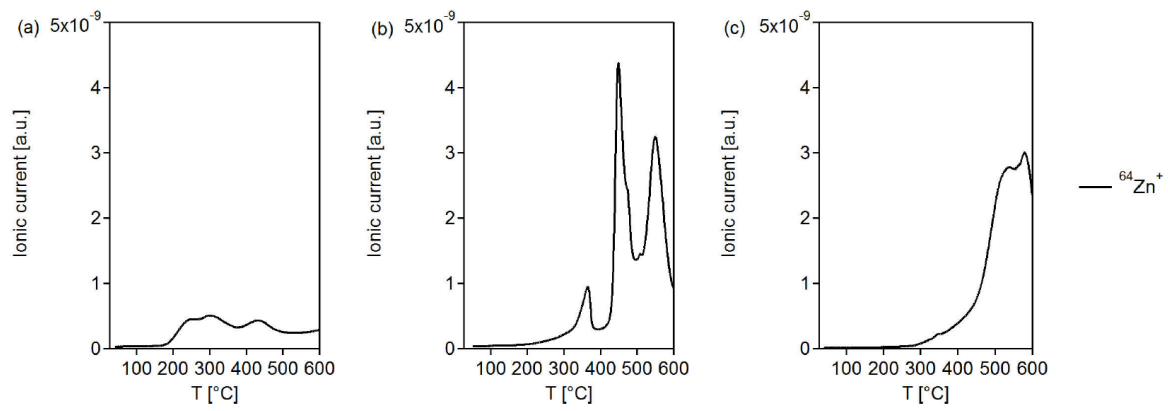


Fig. S5. ^{64}Zn TDS signals for (a) $\text{Si}_{\text{wafer}}/\text{Zn}(1.3\text{nm})/\text{Mo}(3.0\text{nm})$ (b) $\text{Si}_{\text{wafer}}/\text{Zn}(1.6\text{nm})/\text{Ti}(3.3\text{nm})/\text{Mo}(3.0\text{nm})$ and (c) $\text{Si}_{\text{wafer}}/\text{ZnO}(1.8\text{nm})/\text{TiO}_x(4.0\text{nm})/\text{Mo}(3.0\text{nm})$ samples as a function of temperature.

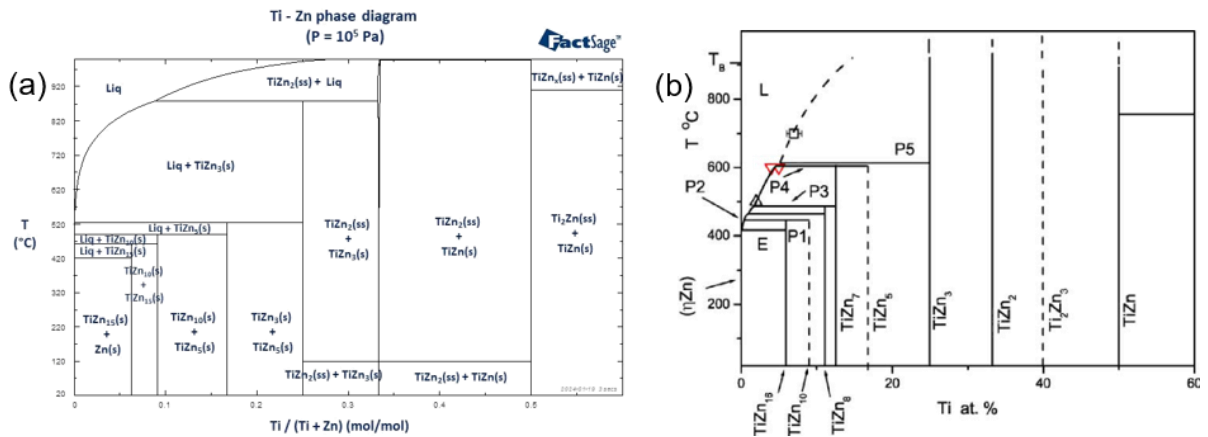


Fig. S6. (a) Ti - Zn phase diagram simulated by *FactSage* software at atmospheric pressure. (b) diagram proposed by Vassilev *et al.* [44].

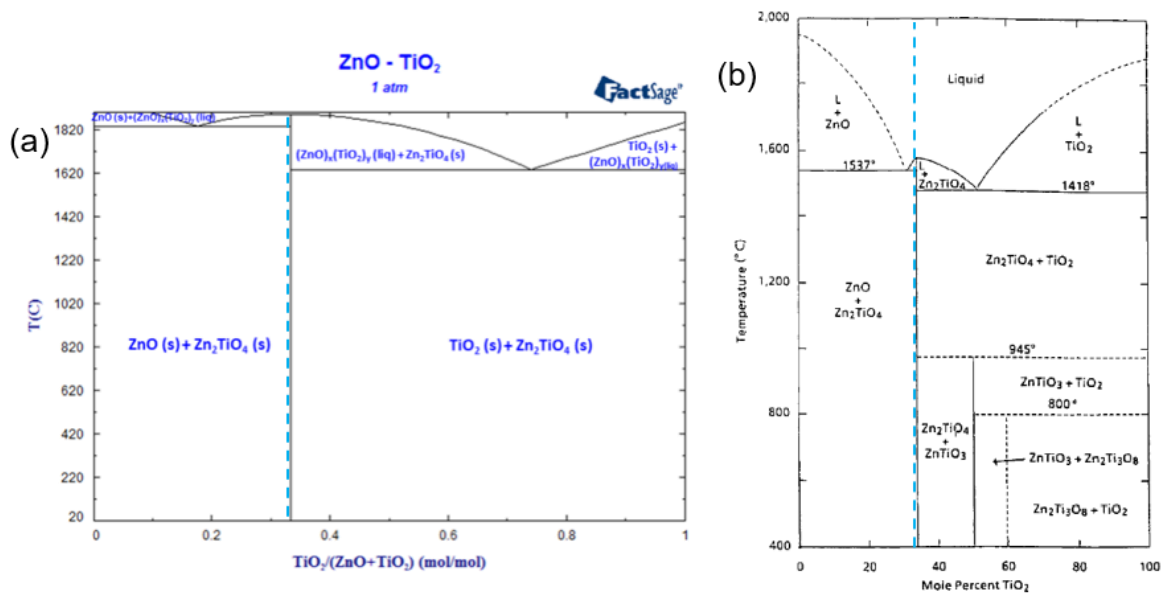


Fig. S7. (a) ZnO-TiO₂ phase diagram simulated by *FactSage* software at atmospheric pressure. (b) diagram proposed by Yang *et al.* [45]. The vertical dotted line corresponds to the molar fraction of 33% of Ti corresponding to film thicknesses ZnO(9.5 nm)/Ti(3.4 nm).

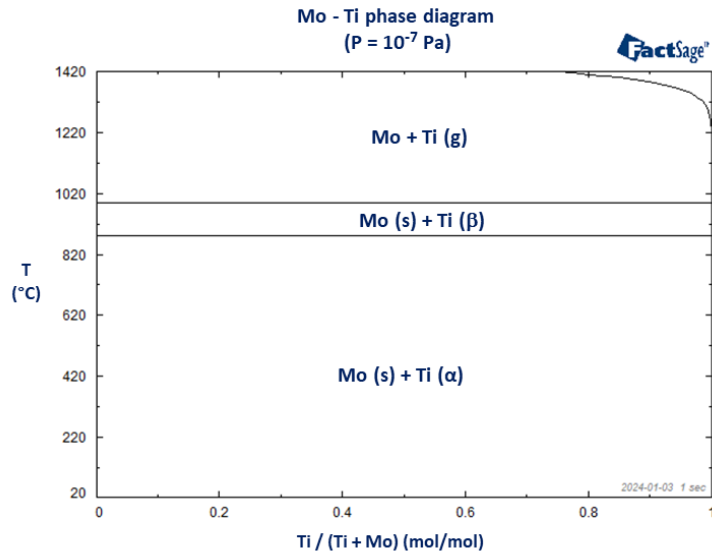


Fig. S8. Mo – Ti phase diagram simulated by *FactSage* software at 10^{-7} Pa.

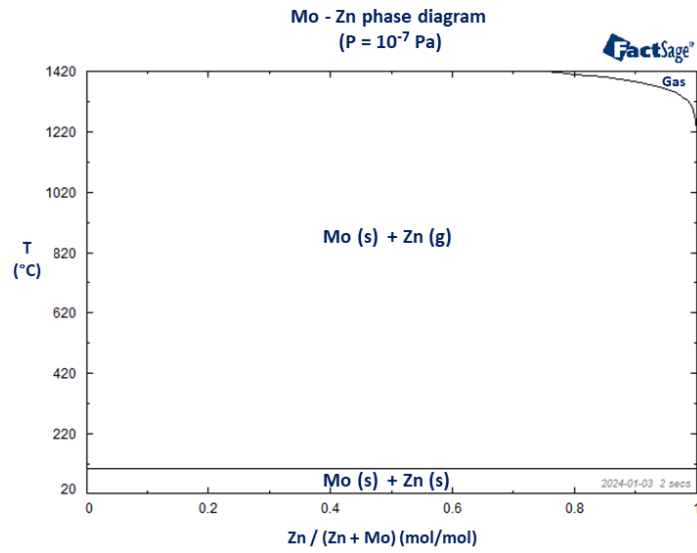


Fig. S9. Zn – Mo phase diagram simulated by *FactSage* software at 10^{-7} Pa.

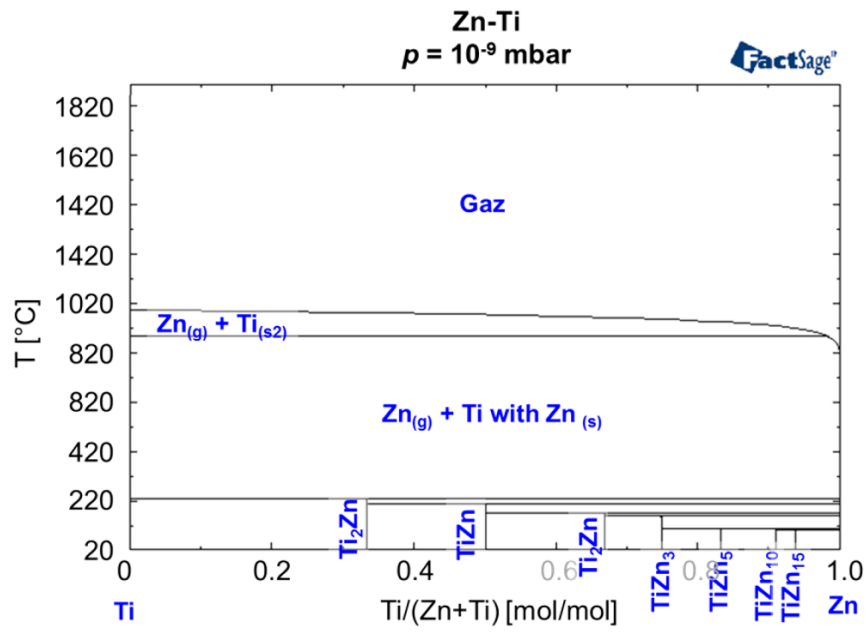


Fig. S10. Ti – Zn phase diagram simulated by *FactSage* software at 10^{-7} Pa.