Re-designing ALD experiments for AI-ready data: The IGZO case study

Supplementary Information

Eleni Poupaki*, Cas Visser, Freek Klabbers, Adrie Mackus, and Erwin Kessels

*Eindhoven University of Technology, Netherlands, *e.poupaki@tue.nl*

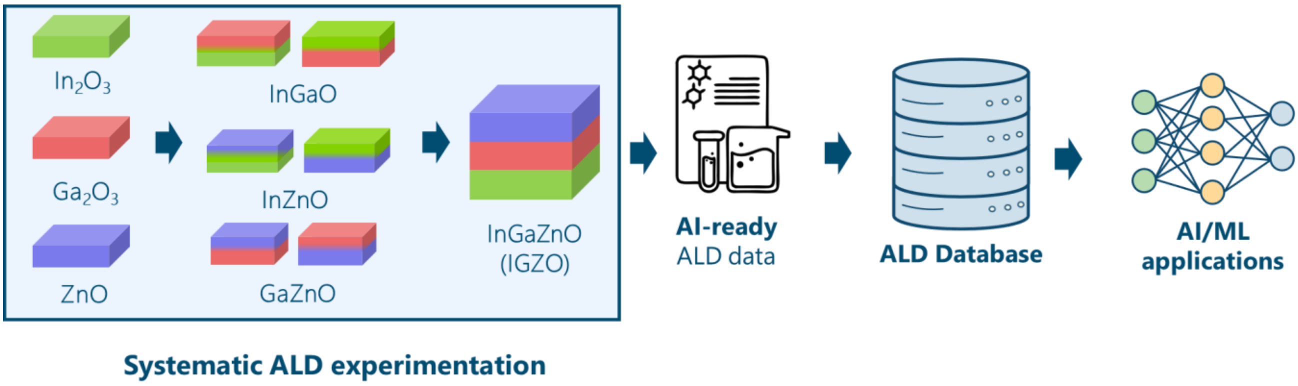

Figure 1: Workflow for building an AI-ready ALD dataset across the In–Ga–Zn–O composition space. Binary ALD processes for In_2O_3, Ga_2O_3, and ZnO are combined through supercycle design recipes to deposit ternary (InGaO, InZnO, GaZnO) and quaternary InGaZnO (IGZO) films. Process parameters and film properties are standardized into an AI-ready format, stored in a centralized ALD database, and used as input for downstream AI/ML applications.

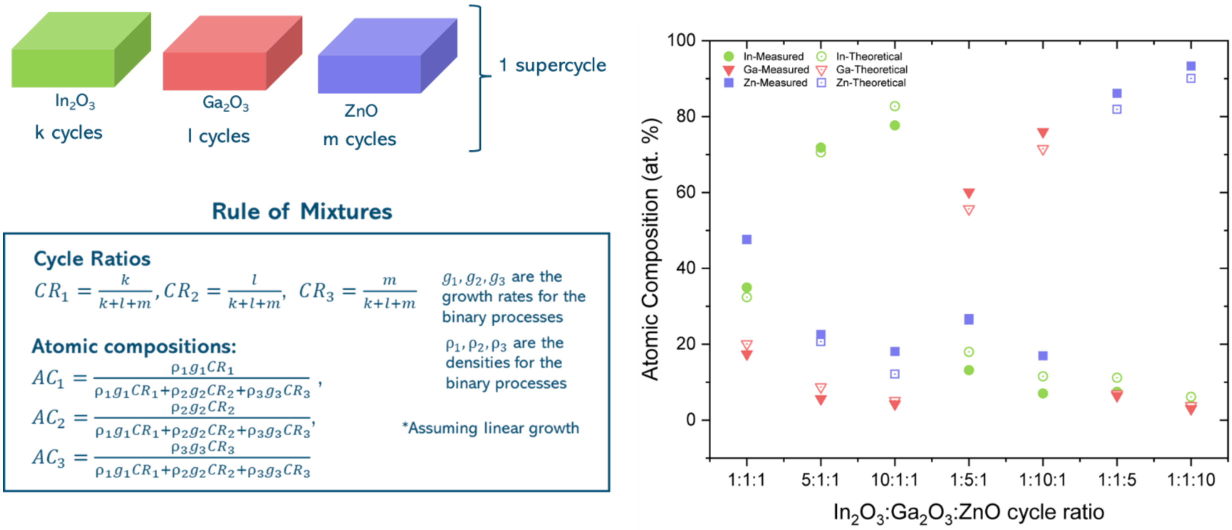

Figure 2: Rule-of-mixtures model for supercycle ALD compositional control. One supercycle combines *k*, *l*, and *m* subcycles of the In_2O_3, Ga_2O_3, and ZnO binary processes; cation fractions AC_i are calculated from the cycle ratios CR_i, binary growth rates g_i, and binary densities ρ_i, assuming linear growth. Measured XPS compositions (filled markers) are compared to theoretical values (open markers) for seven IGZO recipes with In:Ga:Zn cycle ratios of 1:1:1, 5:1:1, 10:1:1, 1:5:1, 1:10:1, 1:1:5, and 1:1:10, confirming control of film composition through the supercycle IGZO recipe.

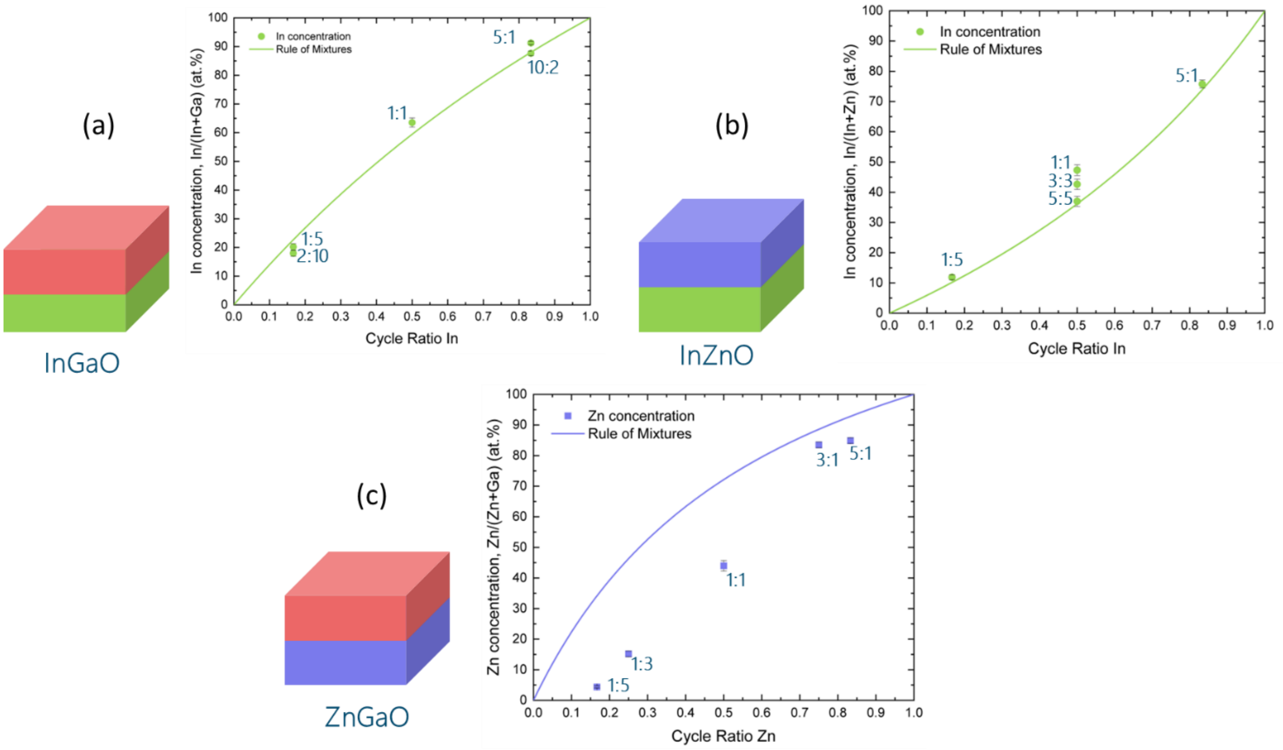

Figure 3: Atomic composition measured from XPS as a function of subcycle ratio for (a) InGaO, (b) InZnO, and (c) ZnGaO, compared to the rule-of-mixtures calculation (solid line; see Fig. 2 for the model). Subcycle ratios are annotated next to each data point. InZnO and InGaO were measured by XPS without sputtering. The lower Zn content in ZnGaO compared to the rule of mixtures reflects preferential Zn sputtering during XPS.