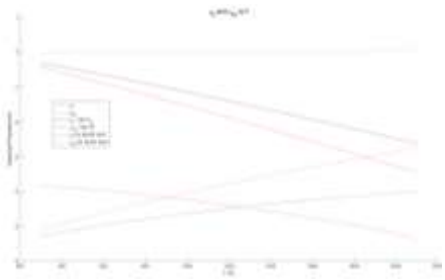

Fig. 1: Ga and O chemical potentials as functions of temperature calculated from thermochemical functions used for Ga-O binary phase diagram for various chemical environments such as: $pO_2 = 10^{-4}$ atm, $pO_2 = 1$ atm, and the equilibrium vapor pressure of Ga over liquid Ga. The non-constant values vs T influence the quantitative defect equilibrium.

Fig. 2: Simplified results for full equilibrium calculation including >350 chargestates of various defects and complexes at different equilibrium temperatures, subject to the constraints that $[Sn_{GaII}] = 2x10^{18}$ /cm^3 but all other Sn-containing defects are set to zero. This illustrates the capability to execute calculations incorporating T-dependent E_c and E_v (which is primarily responsible for suppressing the V_{Ga}), T-dependent chemical potentials, and estimated vibrational entropy, as well as constraints on the concentrations of various defect types.

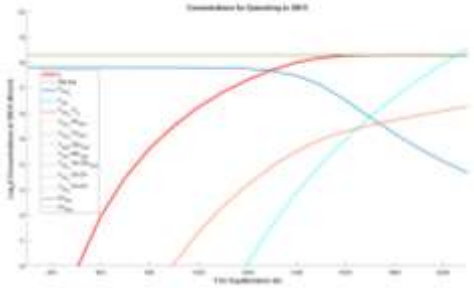

Fig. 3: Simplified results for quenching calculations from the indicated T to 300 K including >350 chargestates of various defects and complexes, subject to the constraints that $[Sn_{GaII}] = 2x10^{18}$ /cm^3 and all other Sn-containing defects set to zero. This illustrates the capability to execute quenching calculations including certain defects constrained to set values.

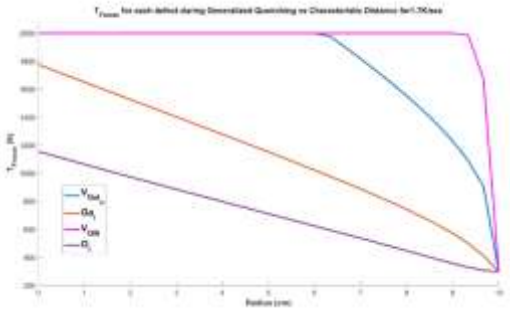

Fig. 3: Illustrative, simplified example of calculated freezing temperatures vs radius in a hypothetical Ga2O3 boule for O_i, Ga_i, relaxed V_{Ga}, and V_{OIII} arbitrarily assigned migration energies of 0.15, 0.2, 0.5, and 0.75 eV as shown.