Modelling of Ga_2O_3 epitaxial phases by first principles calculations

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After reviewing some recent results of ours for relevant surfaces and coherent interfaces of α, β, and κ phases with sapphire (0001), showing that a new reconstruction of the κ (001) surface provides an energy comparable to the one of the β (-2 0 1) surface, we point out that the misfit strain with sapphire overturns the usual hierarchy in cohesion energies of the three phases. This latter issue may be important at the early deposition stages. Then, some results in progress concerning the thermodynamic stability of one α-Ga_2O_3 wetting layer on sapphire and its evolution to plastic (dislocations), or elastic (β islands) relaxation with thickness will be discussed, in connection to existing (and desirable) experimental data. Finally, some exploratory investigations will be reported on the misfit in Bravais cells and the possible structure of Ga_2O_3 interfaces with SiO_x/Si and 3C-SiC/Si, for different orientations and phases.