From sapphire to engineered Si substrates for Ga_2O_3 heteroepitaxy: theory indications to avoid large lattice misfits

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Ga_2O_3 is a promising material for power electronic devices because of the high breakdown voltage, the huge Baliga figure of merit, and the limited thermal budget in deposition: some 500-800 °C, depending on crystal phase and epitaxial method [1]. This latter feature allows for potential integration in the Si technology, but most of the experimental and theoretical studies are focussed in deposition on α-Al_2O_3 (0001) substrates. It is clear that deposition on Si would also be suitable for heat dissipation reasons, as both Ga_2O_3 and Al_2O_3 are poor heat conductors, but some critical issues in Ga_2O_3 heteroepitaxy are present.
The first one is the large polymorphism of Ga_2O_3: β (the monoclinic and stable phase), α (the rhombohedral phase), κ (the orthorhombic phase), δ (the cubic bixbyite phase) and γ (the cubic, defective-spinel phase). The first three polymorphs are the most common ones appearing in heteroepitaxy on sapphire and are really very close in formation energy. [1,2]
The second one is the misfit in symmetry and in lattice parameters, not only with the Si faces, but also with the sapphire substrates, so that rotational domains are quite common in β and κ heteroepitaxy.
The third one is the competing Si oxidation that starts as soon as the oxygen, or water vapor, inlet sets in: either a controlled pre-oxidation is operated (such as the one with ALD or MBE equipment), or an inert buffer layer is deposited (such as 3C-SiC, compatible with Si in deposition temperature).

By a recent first-principles investigation of ours on the volume and surface energies of Ga_2O_3, with and without misfit strain on sapphire (0001) [2], we have shown that the misfit strain alters the hierarchy in energy for differ film phases and orientations, in qualitative agreement to experiments [3]. Calculations of interface energies are in progress, in order to set a quantitative ground for a nucleation and growth modelling of Ga_2O_3 islands [3], but this theoretical background is also used in order to approach the growth of Ga2O3 on SiO_x/Si substrates (thanks to an accurate modelling of the very first stages of Si oxidation, personally communicated by Alfredo Pasquarello and Angelo Bongiorno [4]), and the growth of Ga_2O_3 on 3C-SiC/Si.
We will report about the interfacial matching for different film/substrate orientations, both in terms of lattice misfit and chemical bonding, aiming at providing a systematic roadmap for improving the existing (few) experimental trials, both on Si, or SiO_x/Si, and on 3C-SiC/Si.

References

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