

Chemical vapor deposition (CVD) of polycrystalline SiC for the manufacture of alternative substrates for power electronics application: understanding the process-microstructure-properties relationship

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Abstract : Today, for ecological and geopolitical considerations, we need to reduce our dependence on fossil fuels. To achieve this, a massive electrification of society (industry, transport...) is foreseen. Power devices will play a key role in this transition as they are required for the many power conversions that take place between the production and use of electricity. Silicon carbide's exceptional physical properties make it an ideal material for replacing the silicon commonly used in the manufacture of these devices to improve their performance. However, the manufacture of SiC-based components relies on the availability of large single-crystal substrates of excellent crystalline quality, which are still considered too expensive. A high-potential alternative to conventional substrates consists in transferring a single-crystal thin film onto a polycrystalline SiC receiver, which must be thick, highly conductive (thermal and electrical) and flat. Chemical vapor deposition (CVD) was chosen for the manufacture of these polycrystalline substrates since it enables the growth of dense, thick and doped films along with high throughput. The aforementioned specifications raised new questions of understanding, particularly on the microstructure-properties relationship, but also on the process-microstructure one. The study of these relationships is at the heart of the present thesis and will be addressed by coupling experimental and modeling approaches.

To understand the CVD process, which is inherently multi-physical, simulations based on the finite volume method were used to describe a lab-scale hot wall reactor. A detailed study on heat transfers was carried out and a kinetic model related to deposition in the Si-C-H-Cl system was proposed, showing an excellent agreement with experiments in terms of growth rates over a wide range of process parameters. From these simulations, links between local growth conditions (temperature, species partial pressure) and microstructure of the deposit (grain sizes, preferential orientations)

were formulated and the underlying mechanisms studied. For instance, grain width shows a temperature dependence similar to that governing nuclei density at saturation, suggesting that the first instants of growth partly dictate the evolution of the microstructure. A twin-mediated growth regime operating at low surface supersaturation (high T° , low species partial pressure) and favoring lateral grain growth was also identified and helps explain the formation of preferential orientations along $\langle 110 \rangle$ and $\langle 211 \rangle$. To minimize the resistivity of the deposit, a study of the nitrogen doping of polycrystalline SiC was proposed and has led to the construction of a kinetic doping model of the Si-C-H-Cl-N. From the same study, the resistivity was shown to depend on the doping content but also suggests an effect of grain size, in agreement with models from literature. As the curvature of free-standing films (without substrate) was systematically observed, it was the subject of a dedicated study and was associated with the presence of a stress gradient through their thickness. Two mechanisms were proposed to explain the formation of these gradients, the first being linked to the evolution of grain size through the thickness of the deposit and the second being due to a progressive stress relaxation in the deposit by deformation of the {substrate+layer} system during deposition.

Finally, although this thesis has a strong industrial interest, it was also the opportunity to study innovative scientific issues relating to polycrystalline SiC deposited by CVD.