Simulation of Si Epitaxy in Single Wafer Reactors

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Silicon epitaxy (EPI) is an important process in semiconductor industry. We investigate Si epitaxy using 3D reactor scale computational fluid dynamics simulations coupled with surface chemistry models for the film growth.

In the first part we focus on the deposition of Si and phosphorous-doped Si at low temperature in a simplified reactor geometry. Based on existing DCS-based Si chemistry models [1] for higher process temperatures, we developed a new kinetic chemistry model for lower temperatures [2]. These chemistry models are coupled with CFD based simulations for the gas transport and multi-component diffusion of gas species using the software CFD-ACE+ [3]. This allows for reactor scale process simulations to get a better understanding of the relations between deposited rates and process parameters, enabling rational process optimization, to reduce process variability and to increase within-wafer growth rate homogeneity.

In the second part we introduce our ongoing work on developing a model for a high temperature atmospheric pressure Si epitaxy process using trichlorosilane. Here we investigate the flow field and gas species distribution in a complex 3D reactor geometry using the software COMSOL Multiphysics [4]. The gas mixture consists of hydrogen (H_2) and trichlorosilane (TCS, $SiHCl_3$) with a spatially varying concentration above the rotating wafer. Simulating and visualising the 3D flow field (see Fig. 1) and gas composition is the first step towards an in-depth understanding of the process and optimising it for better homogeneity of the grown layer thickness. We are currently adding radiative, convective and conductive heat transport and we plan to include surface chemistry in the future. This will result in a complete multiphysical model – a digital twin – of this Si-EPI process.

References
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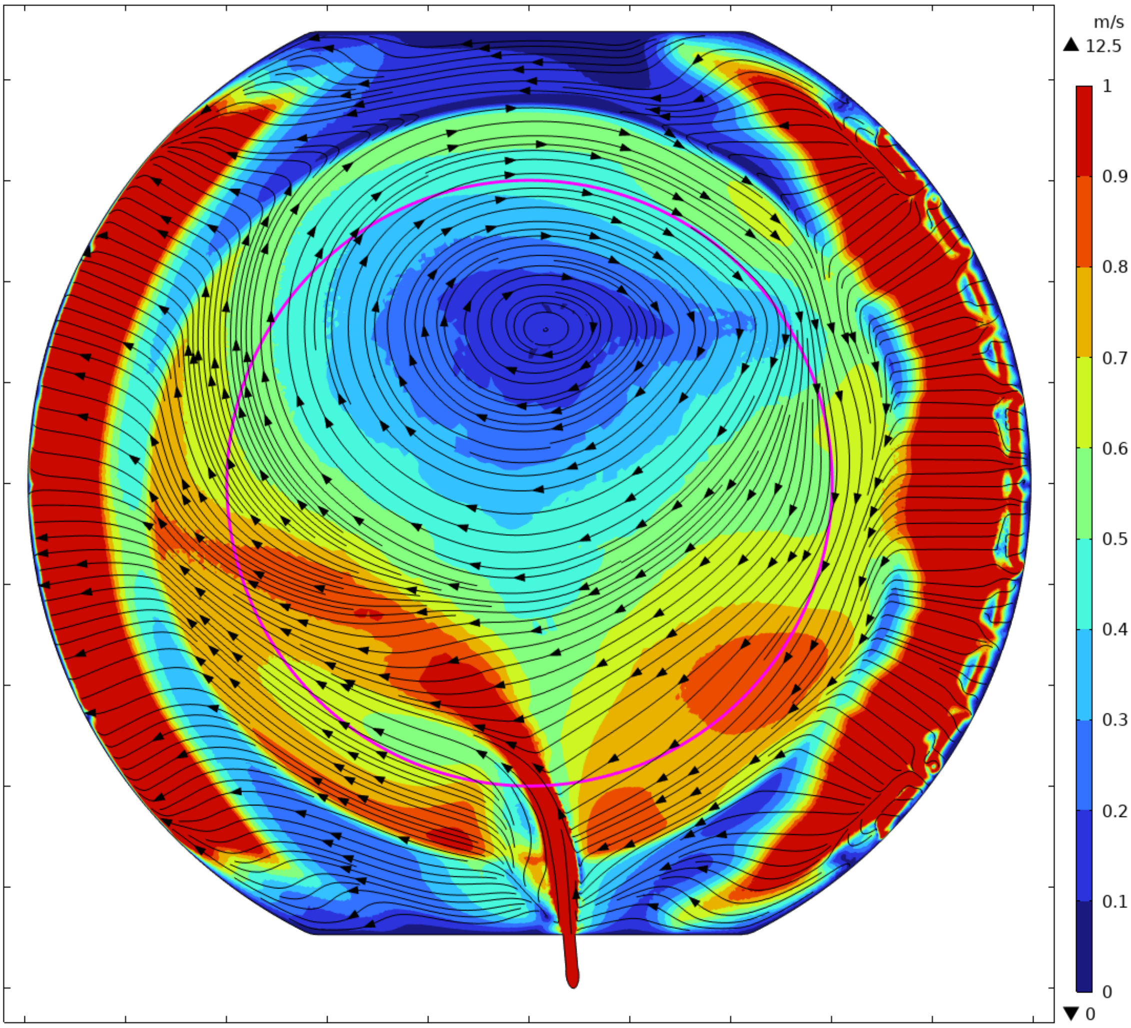

Fig. 1: Gas velocity distribution above a rotating wafer in an atmospheric pressure silicon epitaxy chamber with crossflow using H_2 and TCS.