A fixed point iteration method for multiscale modeling of Chemical Vapor Deposition processes.

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A fixed point iteration method for coupling multiple length scales in Chemical Vapor Deposition (CVD) processes is presented. A Reactor Scale Model (RSM), used for the description of the macro-scale in the bulk, is coupled with a Feature Scale Model (FSM), used for the description of the topography evolution of the micro-scale features on the wafer. The RSM is implemented with a commercial software for computational fluid dynamics, namely FLUENT, and the FSM combines [1] a ballistic model for the species' transport inside features (e.g. trenches), a surface chemistry model, and a profile evolution algorithm based on the level set method. The coupling of the RSM with the FSM is performed through the correction of the boundary condition for the species consumption along the wafer. The pre-exponential factor for the expression of the surface reaction rate is corrected [2] in order for the RMS to take into account the existence of the features in the micro-scale, wihout including them in the computational domain of the macro-scale. The correction is performed through a fixed point iteration method. In the present work the boundness and the stability of the iteration method is studied. Furthermore, the time consuming computations in the micro-scale are sufficiently treated by using parallel processing and Message Passing Interface (MPI) [3].

References

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