A Kinetic Model for Chemical-Vapor Deposition of Pure-Boron Layers from Diborane

V. Mohammadi, W.B. de Boer, T.L.M. Scholtes, L.K. Nanver
Delft Institute of Microsystems and Nanoelectronics (DIMES), Delft University of Technology,
Feldmannweg 17, 2628 CT Delft, The Netherlands,
Phone: +31 (0)15 27 86294, Fax: +31 (0)15 27 87369,
E-mail: v.mohammadi@tudelft.nl

The chemical-vapor deposition of pure boron has in the last years been very successfully applied for fabricating extremely shallow, less than 10-nm deep, silicon p-n junction diodes for a number of leading-edge device applications. This so-called PureB technology has provided particularly impressive performance of photodiode detectors for low penetration-depth beams for which 2-nm-thick PureB-layers are reliably implemented as the front-entrance window [1]. Ideal low-leakage diode characteristics are achieved for deposition temperatures from 400°C - 700°C, which together with the fact that the deposition is conformal and highly selective to Si, also makes PureB technology an attractive candidate for creating junctions on silicon nanowires and advanced CMOS transistors including source/drain in p-type FinFETs [2]. In the latter applications, sub-3-nm thick layers are required to avoid excess series resistance through the high-resistivity boron layer. Therefore, a very good control of the layer thickness is crucial.

In this paper, an analytical model is established to describe the deposition kinetics and the deposition chamber characteristics that determine the deposition rate over the wafer. The predictive capabilities of the model have been verified by experiments, performed at 700 °C in different ASM CVD reactors.

Prior models can be divided into two main groups. The first covers models that has been developed on the basis of the boundary layer theory and only consider physical diffusion effects [3]. The second encompasses models that consider the surface reactions [4]. In contrast, our kinetic model is developed to predict the deposition rates of PureB-layers on a non-rotating silicon wafer. The model takes into consideration the diffusion mechanism of the diborane species through the stationary boundary layer over the wafer, the gas phase processes and the related surface reactions by applying the actual parabolic gas velocity and temperature gradient profiles in the reactor which were calculated theoretically and also simulated with FLUENT® software. Starting point for developing a mathematical model for the chemical and physical behavior of the CVD process is the expression for the temperature and velocity profile for a fully-developed flow which can be calculated by solving the equation for energy conservation, the continuity equation and the equation of motion for the carrier gas:

\[ \frac{c_v \rho \partial T}{\partial x} = \frac{\partial}{\partial x} \left( \frac{k_x}{\mu c_p} \frac{\partial T}{\partial x} \right) = 0 \]  \hspace{1cm} (1)

\[ \frac{\partial \rho u}{\partial y} = \text{constant} \]  \hspace{1cm} (2)

where \(c_v\), \(\rho\), \(\mu\), \(c_p\), \(k_x\) and \(T\) are the gas velocity profile, axial position in the direction of the gas flow, temperature-dependent thermal conductivity and dynamic viscosity of the carrier gas, respectively. The solution of these equations leads to a distorted parabola with its maximum shifted towards the colder part of the reactor, and the gradually decreasing temperature above the susceptor, which are confirmed by simulation results. Consequently, the velocity of gas molecules is different at gas boundaries where the vertical diffusion of gas molecules occurs. This effect was also considered in the implementation of the model.

This model is based on a wide range of input parameters, such as initial diborane partial pressure, total gas flow, axial position on the wafer, deposition temperature, activation energy of diborane deposition, surface H-coverage and reactor dimensions. By only adjusting these reactor-specific parameters, this model was also successfully transferred from the ASM Epsilon One to the Epsilon 2000 reactor which has totally different reactor conditions. In fact, this model has the capability to predict the deposition rate on any 2-D uniform or non-uniformly patterned wafer such as those used for advanced device fabrication.

In Fig. 1 several experiments results are compared to model predictions made without fitting. The PureB deposition rates are extracted as a function of (a) an axial position, \(x\), for different gas flow and diborane partial pressure conditions, (b) gas flow over the susceptor, and (c) diborane partial pressure including curves for two different axial positions. Experimental and predicted results for ASM Epsilon 2000 are also shown. A very small, less than 5%, deviation between experimental results and model prediction is plausibly related to the lateral diffusion of the diborane atoms and it becomes more evident at lower gas flows and diborane partial pressures.

![Figure 1. Model and experimental results for the PureB deposition rate as a function of (a) an axial position, x, (b) main gas flow over the susceptor, and (c) diborane partial pressure. The applied diborane partial pressures were 3.39, 2.55 and 1.7 mtorr given by P1, P2 and P3, respectively. And the applied gas flows were 20, 15 and 10 slm given by F1, F2 and F3, respectively. All experiments were performed at atmospheric pressure.](image-url)

It can be concluded, that the data calculated on the basis of this model fits well with the experimental results and it has been very useful in the development of uniform PureB-layers with little pattern dependence as well as for transferring recipes from one reactor to the other. The deposition of 2-nm-thick PureB-layers with only a few angstrom thickness variations is now performed standardly for a variety of process wafer conditions.