A KINETIC MODEL FOR P-TYPE DOPING IN SILICON EPITAXY BY CVD

Bhavesh Mehta and Meng Tao*
NanoFAB Center and Department of Electrical Engineering, University of Texas at Arlington
500 S. Cooper St., Arlington, Texas 76019
*mtao@uta.edu

A kinetic model based on 1) the collision theory of heterogeneous unimolecular elementary reactions, 2) statistical physics, and 3) the concept of competitive adsorption is proposed for p-type doping in Si epitaxy by chemical vapor deposition (CVD). The model takes into account an extensive set of elementary heterogeneous reactions, which involves two precursors, SiH_4 and B_2H_6, and four types of surface sites, H-terminated Si and B sites and H-free Si and B sites. The resultant eight reactions are listed in Table 1. The activation energies for reactions on H-terminated Si and B sites are larger and therefore these fluxes can be neglected as compared to those on H-free Si and B sites. The model provides analytical equations to describe p-type carrier concentration and growth rate as a function of deposition conditions including temperature and partial pressure of dopant precursor. At low temperatures, the enhancement in growth rate with B_2H_6 partial pressure is attributed to enhanced H desorption from B sites as compared to Si sites, which act as catalytic sites for Si growth (Fig. 1). Although B concentration shows a linear dependence on B_2H_6 partial pressure, the relationship is more complicated. The apparent linearity is a combined effect of non-linear B growth rate and non-linear Si growth rate (Fig. 2). At low temperatures, $J_{BH_3 \text{ on } Si}$ is the dominating B flux at low B_2H_6 partial pressures, whereas $J_{BH_3 \text{ on } B}$ dominates at high B_2H_6 partial pressures. At temperatures >750°C, $J_{BH_3 \text{ on } B}$ does not play much role in B growth. The model agrees well with the experimental data for p-type doping in silicon epitaxy.

1. D.A. Grutzmacher, J. Cryst. Growth 182, 53 (1997).

Table 1. Heterogeneous chemical reactions involved in p-type doping in Si epitaxy using SiH_4 and B_2H_6

Flux	Reaction
$J_{SiH_4 \text{ on } Si}$	$SiH_4(g) + 2\text{-}Si(s) \rightarrow H_3Si\text{-}Si(s) + H\text{-}Si(s)$
$J_{SiH_4 \text{ on } H\text{-}Si}$	$SiH_4(g) + H\text{-}Si(s) \rightarrow H_3Si\text{-}Si(s) + H_2(g)$
$J_{SiH_4 \text{ on } B}$	$SiH_4(g) + \text{-}B(s) + \text{-}Si(s) \rightarrow H_3Si\text{-}B(s) + H\text{-}Si(s)$
$J_{SiH_4 \text{ on } H\text{-}B}$	$SiH_4(g) + H\text{-}B(s) \rightarrow H_3Si\text{-}B(s) + H_2(g)$
$J_{BH_3 \text{ on } Si}$	$BH_3(g) + 2\text{-}Si(s) \rightarrow H_2B\text{-}Si(s) + H\text{-}Si(s)$
$J_{BH_3 \text{ on } H\text{-}Si}$	$BH_3(g) + H\text{-}Si(s) \rightarrow H_2B\text{-}Si(s) + H_2(g)$
$J_{BH_3 \text{ on } B}$	$BH_3(g) + \text{-}B(s) \rightarrow H_2B\text{-}B(s) + H\text{-}Si(s)$
$J_{BH_3 \text{ on } H\text{-}B}$	$BH_3(g) + H\text{-}B(s) \rightarrow H_2B\text{-}B(s) + H_2(g)$

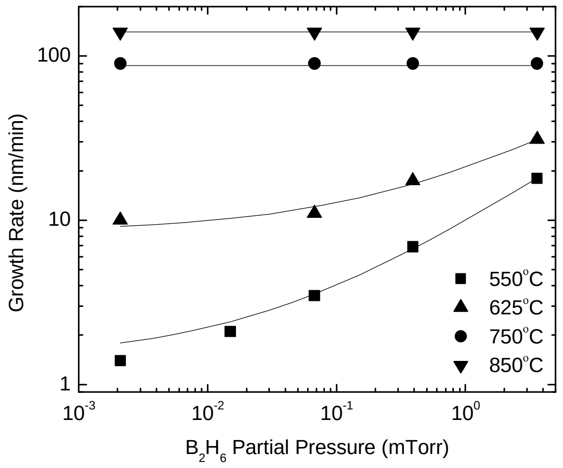

Fig. 1. Dependence of growth rate on B_2H_6 partial pressure in the temperature range of 550–850°C. Solid lines are from our model and data points from Ref. 1.

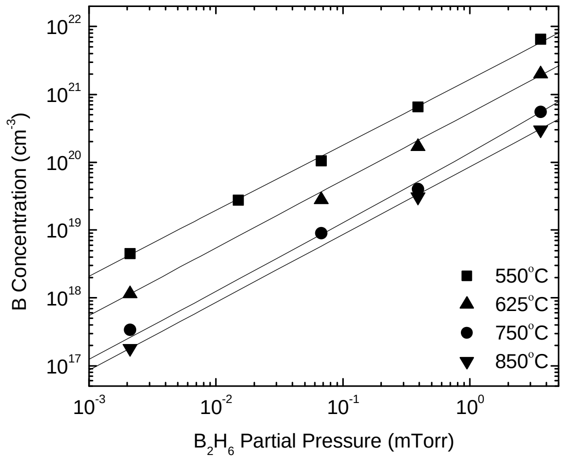

Fig. 2. Dependence of B concentration on B_2H_6 partial pressure in the temperature range of 550–850°C. Solid lines are from our model and data points from Ref. 1.