

# Investigation of the passivation of $p$ -type dopants by hydrogen in silicon carbide using computational modeling

Bálint Aradi

## Theses:

1. I have shown that the interstitial hydrogen behaves as a very shallow donor in  $3C$ -SiC, while it is an amphoteric trap with negative  $U$  behavior in  $4H$ -SiC. The interstitial hydrogen is positively charged in  $p$ -type doped material in both polytypes, which promotes the forming of complexes between the negatively charged acceptors and the hydrogen.
2. I have calculated the energetics of the interactions between the hydrogen and the silicon and carbon vacancies in  $4H$ -SiC. According to my results, the effective activation energy of hydrogen in radiation damaged samples is between 3,5 and 5,3 eV depending on the Fermi-level. This fits well to the experimental values between 3,5 and 4,9 eV.
3. I have calculated the amount of incorporated hydrogen during different environmental conditions with technological relevance. I could give an estimation to the hydrogen incorporation efficiency of the different methods. I have shown, that in  $p$ -type samples the positively charged hydrogen is the dominating form of hydrogen, while in  $n$ -type samples the  $V_{Si} + 2H$  dominates. I have shown that the amount of incorporated hydrogen in the CVD grown  $n$ -type samples is below the detection limit which is in accordance with the experimental observations. I have shown, that the concentration of the directly incorporated hydrogen molecules is negligible, but at a Fermi level of  $E_F \approx E_V + 2,2$  eV molecules can be formed from interstitial hydrogen atoms.
4. I have shown, that the diffusion of the positively charged hydrogen has a barrier of 0,4 eV in intrinsic material without radiation damages, which implies that the hydrogen is very mobile at the usual growing temperatures (1500°C).
5. I have shown, that the substitutional boron and aluminum which give rise to  $p$ -type acceptors, form electrically inactive complexes with the interstitial hydrogen in silicon carbide. This explains the decrease of the free carrier concentration after the hydrogen annealing of silicon carbide. The calculated dissociation energies of the stable  $B + H$  and  $Al + H$  complexes (2,4 and 1,5

eV) are in good agreement with experimental measured values (2,4 and 1,6 eV). The difference between the two cases can be explained by the different stable configurations. With the help of the dissociation energies I could explain the observed effective activation energy of the diffusion of hydrogen in *p*-type samples.

6. I have shown, that during the CVD growth boron – in contrast to aluminum – is not incorporated atomic but in the form of B + H complexes into silicon carbide. This explains, why the amount of incorporated hydrogen is equal to that of the incorporated boron in boron doped CVD grown samples, and why is it about two orders of magnitude less than that of the incorporated aluminum in aluminum doped samples.
7. I have shown, that the presence of hydrogen determines the activation energy of the incorporated boron acceptors. Boron prefers the silicon site in the presence of hydrogen, while in the absence of hydrogen it prefers the carbon site. This explains the observed fact that implantation produces deep boron acceptors, while doping during growth leads to shallow boron acceptors.