Numerical Study of Bloch Electron Dynamics in Wide Band-Gap Semiconductors

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INTRODUCTION

- A numerical study of the Bloch electron (hole) dynamics in 4H-SiC, 3C-SiC and wurtzite GaN is presented.
- The calculation is based on a 3-band k·p model including spin orbit interaction, where the band structure parameters have been obtained from ab initio band structure calculations.
- The interband tunneling at different electric fields have been calculated around the maximum of the valence band structure where bands are close together in energy.

RESULTS

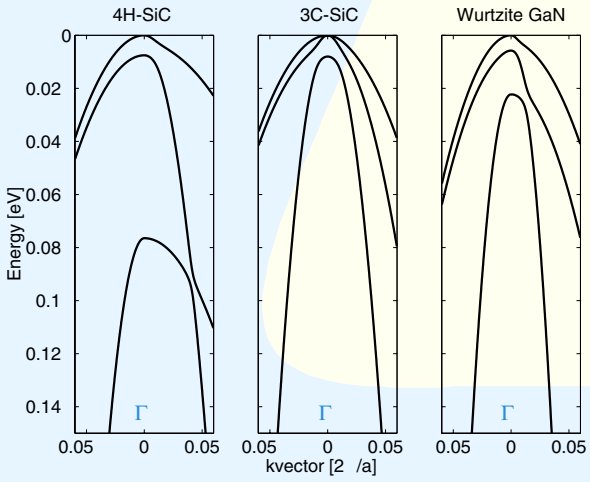

Fig 1. K·p band structures. 4H-SiC and W-GaN: $k_{\perp c\text{-}axis}$ is in the positive direction and $k_{//c\text{-}axis}$ is in the negative direction. 3C-SiC: $k_{\Gamma L}$ is in the negative direction and $k_{\Gamma X}$ is in the positive direction.

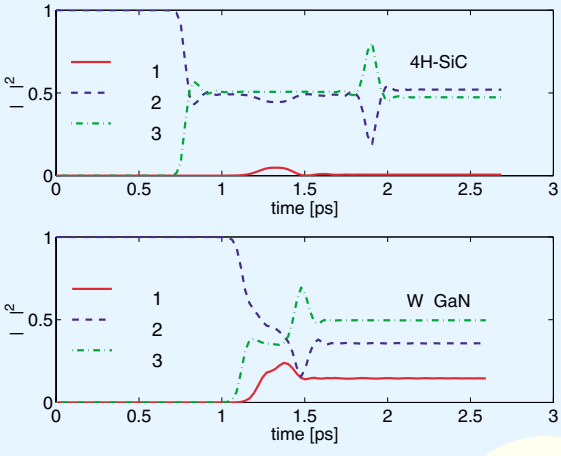

Fig 2. Time evolution of the probability to find the hole in different bands along the c-axis close to the Γ-point. The electric field is 10 kV/cm.

- Significant tunneling between bands occur in 4H-SiC and wurtzite GaN at an electric field as low as 10 kV/cm.
- Interband tunneling is found to be present in 3C-SiC at an electric field of 40 kV/cm applied along the Γ-L segment.
- A smaller energy separation between bands provides stronger tunneling (see Fig. 4. and 5.).
- The tunneling is very weak for smooth bands while it becomes strong in regions where the curvature changes rapidly.

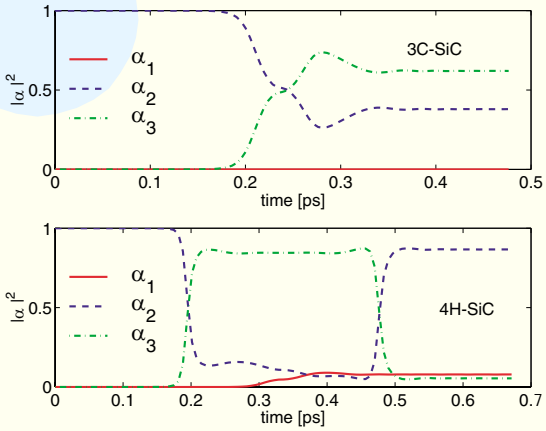

Fig 3. Time evolution of the probability to find the hole in different bands for a drift in 3C-SiC (along the Γ-L segment) and 4H-SiC (along the c-axis). The electric field is 40 kV/cm.

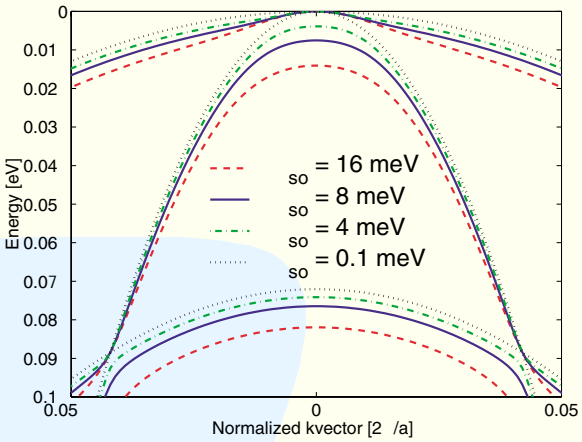

Fig 4. Energy dispersion along the c-axis in 4H-SiC for different spin orbit split Δ_{so}.

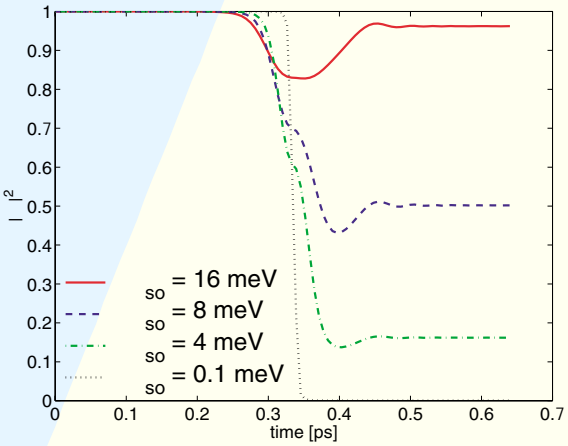

Fig 5. Time evolution of the probability find the hole in band 1 during a drift along the c-axis in 4H-SiC for different spin orbit split Δ_{so}.

- The interband tunneling is expected to influence the transport properties at
  - ⇒ low temperatures where the average time between scattering is large.
  - ⇒ high fields where the hole may drift long distances in k-space between scattering events.