Energetics and Migration of Defects in Germanium

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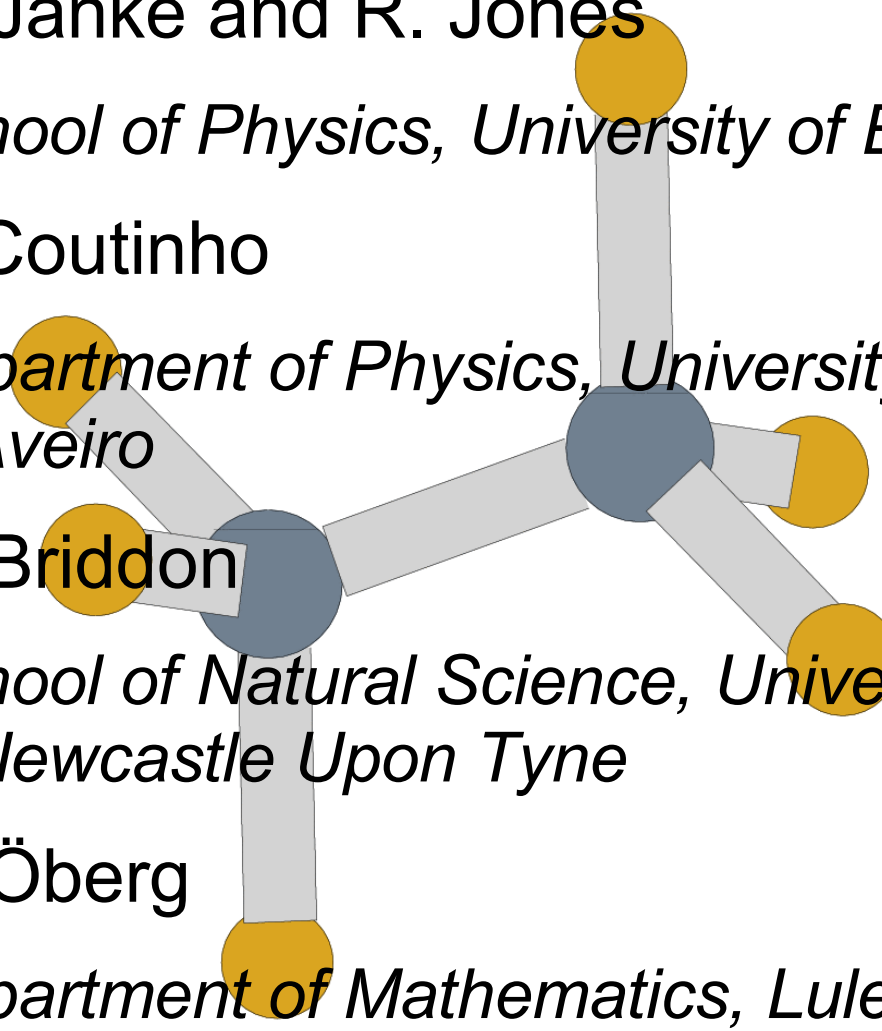

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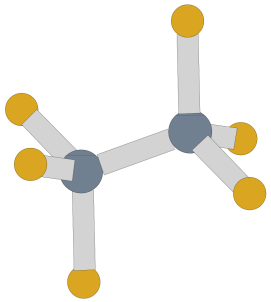
Overview



- Background
- Method
- Divacancies
  - L-point sampling
  - Migration Barriers
- Boron
  - Diffusion methods
  - Migration barriers
  - Further Work

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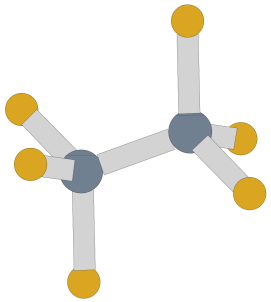
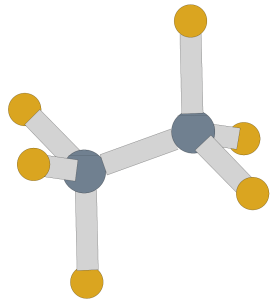
Background

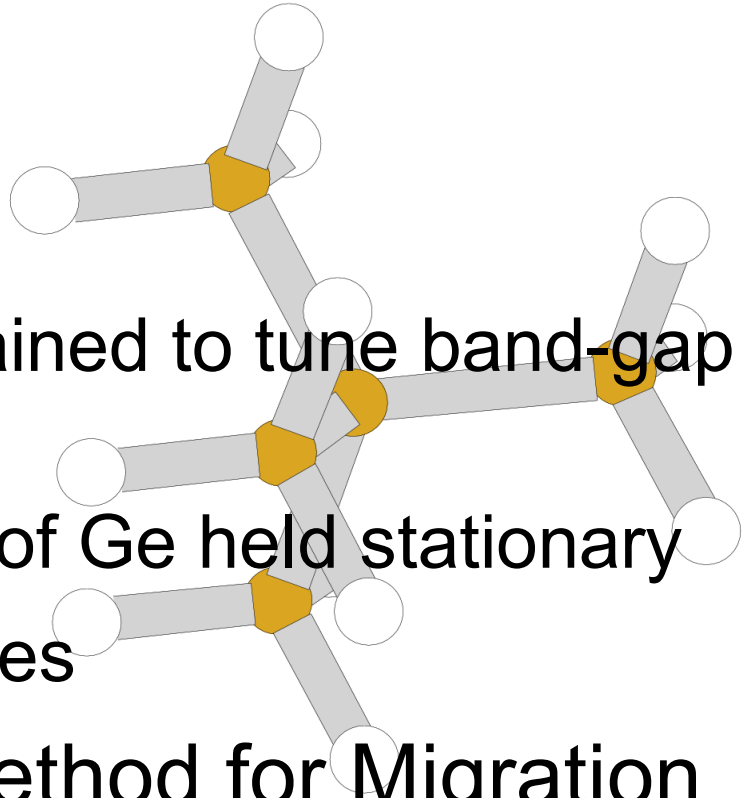


- Vacancy-induced effects of Ge device performance
  - Diffusion - vacancies mediate diffusion
  - Voids - due to vacancy clustering (Hens, 2005)
- Boron - p-type dopant. Different behaviour from Si case - no enhanced diffusion

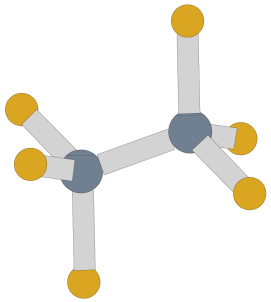
Theoretical method



- Density Functional Theoretical Calculations
  - Local Density Approximation
  - AIMPRO
- 216 atom supercell
  - neutral state
- 501 atom cluster
  - Surface H-Ge bonds strained to tune band-gap or relaxed
  - H atoms and outer shell of Ge held stationary
  - required for charged states
- Nudged Elastic Band method for Migration



Divacancy - Experimental Data



- Mooney 1983
  - Transient Capacitance Spectroscopy
  - Divacancy (Ec-0.32&0.35) in Ge stable up to 150ºC
- Fage-Pedersen 2000
  - Deep Level Transient Spectroscopy measurements
  - Divacancy (Ec-0.29eV) in Ge stable up to 180ºC

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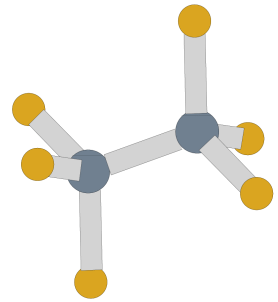
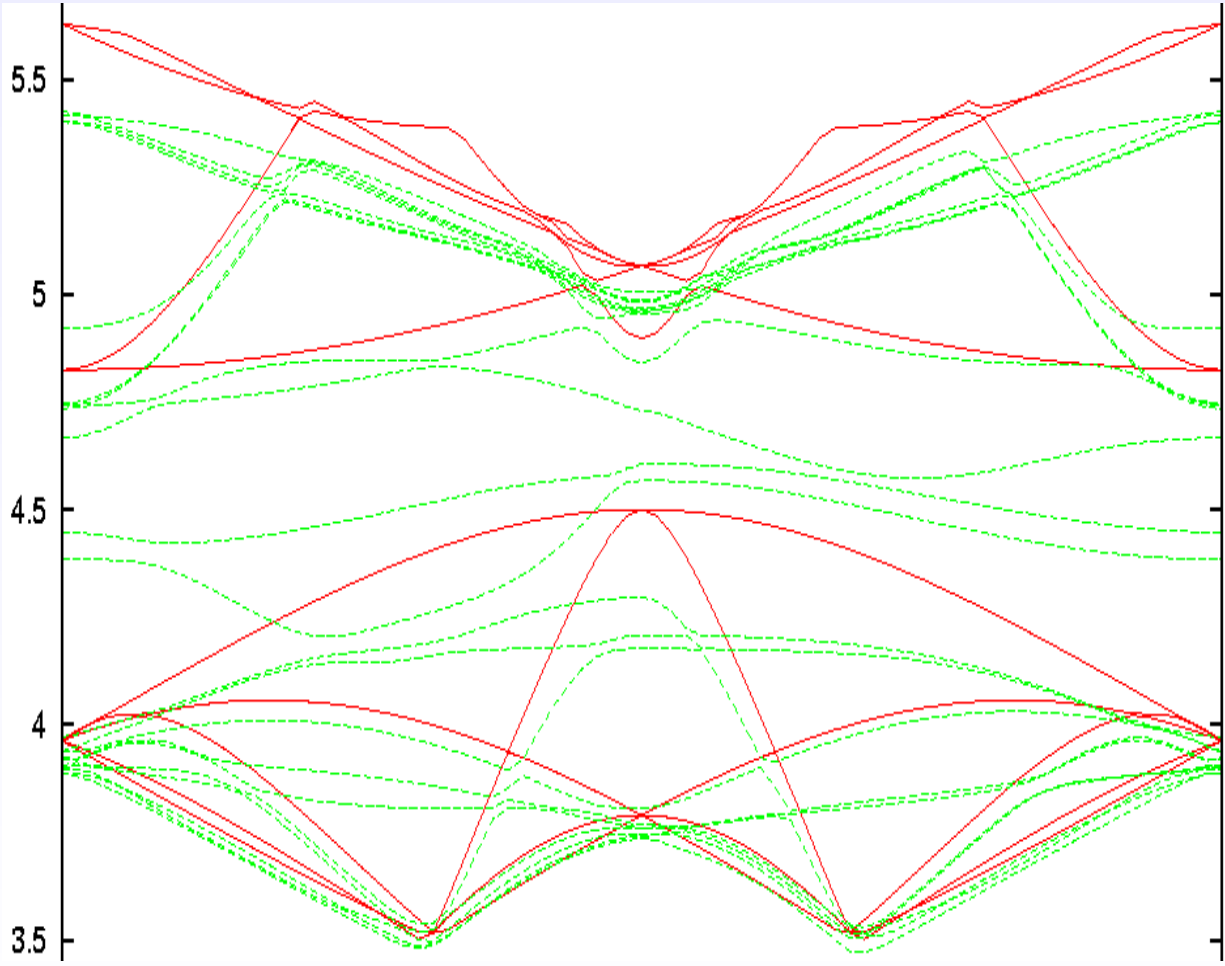
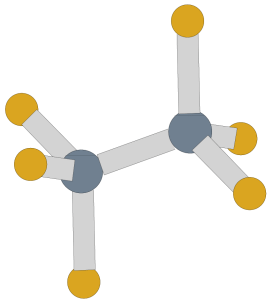
Divacancies - L-point Sampling



- Small Ge band-gap leads to problems with charge states and energy levels.
- MP222 - slightly larger gap, but energy levels are complicated here.
- L-point - larger band-gap, and energy levels cleaner

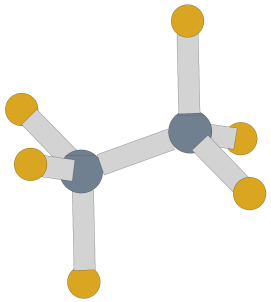


Divacancies - Supercell Results



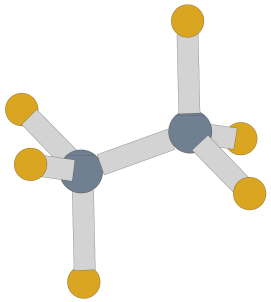
- Divacancy in Ge - MP-2^3 sampling
  - Binding Energy: 0.7 eV
  - Migration Energy 0.7 eV
- Divacancy in Ge - L-point sampling
  - Binding Energy: 1.1 eV
  - Migration Energy: 0.7 eV

Divacancies - Cluster Results



- Migration Energy: 1.0 eV (singly positive V2) to 1.3 eV (doubly negative V2)
- Binding Energy: 1.5 eV (neutral V2) to 1.6 eV (doubly negative V2)
- Migration Energy seen to be independent of surface conditions. Binding energy slightly increases with relaxed Ge-H bonds.

Divacacny - Summary



- Supercell
  - ~0.7 eV migration energy for both sampling methods
  - low thermal stability (Tc~255K)
- Cluster
  - ~1.0-1.3 eV migration energy
  - higher thermal stability closer to experiment (Tc~390 (neutral) -580K (doubly negative))
- Bandstructure analysis casts doubt on supercell results. Binding energies probably somewhere between.

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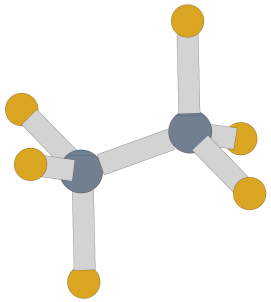
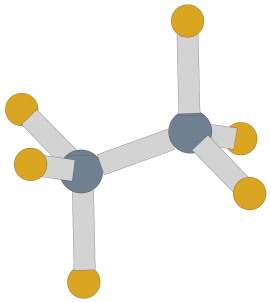
Boron - Diffusion Methods



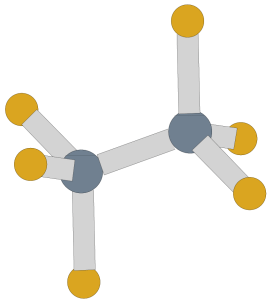
- Vacancy Mediated Diffusion
  - Vacancy Formation Energy
  - Vacacny-Boron Binding and Exchange Energies
- Self-Interstitial Mediated Diffusion
  - Self-Interstitial Formation Energy
  - Self-Interstitial-Boron Binding and Kick-Out, and Interstitial Boron Diffusion Energies
- Concerted Exchange
  - Germanium-Boron Exchange Energy.

Boron - Vacancy Mediation



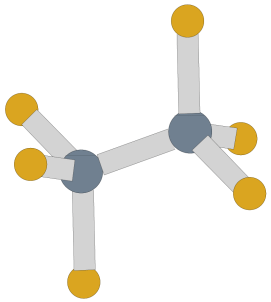
- Vacancy Formation Energy: 2.5 eV
- Cluster BV Binding energy: 0.1 eV
- Supercell BV Binding Energy: -0.3 (L-point), -0.5 (MP-2^3)
- Structure:
  - Cluster - Expanding V, contracting B
  - Supercell - Contracting V and B
  - Cluster results due to fixed volume.
- BV not bound - not a favourable process

Boron - Interstitial Mediation



- Self-Interstitial Formation Energy 3.6 eV (T-site)
- Self-Interstitial-Boron Binding Energy 1.0 eV
- Kick-Out Barrier, and Interstitial Boron Migration Energy to be calculated.
- Self-Interstitial Formation Energy High
  - Very few interstitials present to fuel process

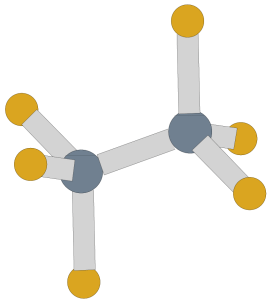
Boron - Concerted Exchange



- Supercell Barrier: 4.2 eV (neutral)
  3.5 eV (singly negative)
- Cluster Barrier: 3.8eV (neutral)

- Work in Progress

Boron - Summary



- Experimental Data - Boron diffuses under annealing at 875ºC for 12 hours (Uppal 2004).
  - suggests a barrier of ~3 to 3.3 eV
- Vacancy mediation
  - BV not bound.
  - Fixed volume in cluster disturbs results
- Interstitial Mediation
  - Interstitial formation energy very high (3.6 eV)
- Concerted Exchange
  - High Barrier (3.5-4.2 eV)

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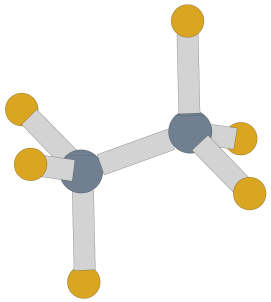
Boron - Further Work



- Concerted Exchange:
  - Calculate Singly Negative Cluster Barrier
  - Further Investigate Supercell Barriers
- Interstitial Mediation:
  - Calculate Kick-Out Barrier and Diffusion Barrier for Boron Interstitial

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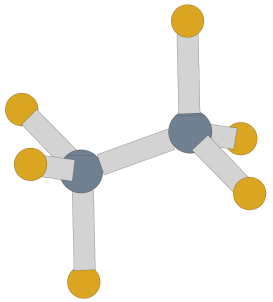
Thank you for listening



Questions?