

# DENSITY FUNCTIONAL THEORY MODELLING OF INTRINSIC AND DOPANT-RELATED DEFECTS IN GE AND SI

Submitted by Colin Janke to the University of Exeter as a  
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## Abstract

This thesis covers the application of the local density approximation of density functional theory to a variety of related processes in germanium and silicon. Effort has been made to use calculated results to explain experimentally observed phenomena.

The behaviour of vacancies and vacancy clusters in germanium has been studied as these are the dominant intrinsic defects in the material. Particular attention was paid to the annealing mechanisms for the divacancy as a precursor to the growth of the larger clusters, for which the electrical properties and formation energies have been studied. Some preliminary work is also presented on the germanium self-interstitial structure and migration paths.

Attention was then turned to a selection of dopant-vacancy defects in both silicon and germanium. An effort was made to explain recent experimental observations in silicon through investigating a number of defects related to the arsenic E-centre. Following this, the properties of donor-vacancy clusters in germanium were studied, and comparison with the results calculated for silicon suggest a significant parallel between the behaviour of the defects and dopants in the two materials.

Finally, extensive work was performed on the diffusion of phosphorus and boron in germanium. Diffusion of both dopants was studied via interstitial and vacancy mediated paths as well as by a correlated exchange path not involving any intrinsic defects. The results obtained confirmed current theories of the mechanisms involved in the diffusion of the two defects, while also expanding the knowledge of other paths and giving Fermi level dependences for the energy and mechanism for diffusion of the two defects. Boron diffusion was found to exhibit strong Meyer-Neldel rule effects, which are used to explain the unusually high diffusivity prefactors and energy barriers calculated from experimental measurements for this dopant.

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# List of Publications

## First Author

1. *Supercell and cluster density functional calculations of the thermal stability of the divacancy in germanium*  
C. Janke, R. Jones, J. Coutinho, S. Öberg and P. R. Briddon, Mat. Sci in semicond. Proc. **9**, 484 (2006)
2. *Ab initio investigation of boron diffusion paths in germanium*  
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3. *Supercell and cluster density functional calculations of the thermal stability of the divacancy in germanium*  
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4. *Ab initio studies of arsenic and boron related defects in silicon mesa diodes*  
C. Janke, R. Jones, S. Öberg and P. R. Briddon, Appl. Phys. Lett **90**, 152103 (2007)
5. *Ab initio investigation of boron diffusion paths in germanium*  
C. Janke, R. Jones, S. Öberg and P. R. Briddon, Phys Rev B, **77**, 075208 (2008)
6. *Ab initio investigation of phosphorus diffusion paths in germanium*  
C. Janke, R. Jones, S. Öberg and P. R. Briddon, Phys Rev B, **77**, 195210 (2008)

7. *Ab initio investigation of phosphorus and boron diffusion in germanium*

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## Collaborative Work

1. *Early stage donor-vacancy clusters in germanium*

J. Coutinho, V. J. B. Torres, S. Öberg, A. Carvalho, C. Janke, R. Jones and P. R. Briddon, *J. Mater. Sci: Mater. Electron.*, **18**, 769 (2006)

2. *Strong compensation of n-type Ge via formation of donor-vacancy complexes*

J. Coutinho, C. Janke, A. Carvalho, V. J. B. Torres, S. Öberg, R. Jones and P. R. Briddon, *Phys. B*, **401**, 179 (2007)

3. *Self-interstitial in germanium*

A. Carvalho, R. Jones, C. Janke, J. P. Goss, P. R. Briddon, J. Coutinho, S. Öberg, *Phys. Rev. Lett.*, **99**, 175502 (2007)

4. *Limits to n-type doping in Ge: Formation of donor-vacancy complexes*

J. Coutinho, C. Janke, A. Carvalho, S. Öberg, V. J. B. Torres, R. Jones, P. R. Briddon, *Defects and Diffusion Forum*, **273**, 93 (2008)

5. *Primary defects in n-type irradiated germanium: a first-principles calculation*

A. Carvalho, R. Jones, C. Janke, S. Öberg and P. R. Briddon, *Sol. Stat. Phen.*, **131-133**, 253 (2008)

6. *First-principles study of the diffusion mechanisms of the self-interstitial in germanium*

A. Carvalho, R. Jones, J. P. Goss, C. Janke, S. Öberg and P. R. Briddon, *J. Phys.: Cond. Mat.*, **20**, 135220 (2008)

# Contents

<b>Abstract</b>	<b>ii</b>
<b>Acknowledgements</b>	<b>iii</b>
<b>List of Publications</b>	<b>iv</b>
<b>List of Figures</b>	<b>xii</b>
<b>List of Tables</b>	<b>xv</b>
<b>1 Introduction</b>	<b>1</b>
1.1 Introduction . . . . .	1
1.2 Silicon and Germanium . . . . .	1
1.3 Unintentional Defects . . . . .	3
1.3.1 Intrinsic Point Defects . . . . .	3
1.3.2 Dislocations . . . . .	10
1.3.3 Donor-Vacancy Complexes . . . . .	11
1.4 Doping . . . . .	13

1.4.1	Implantation of Dopants . . . . .	13
1.4.2	Dopant Activation . . . . .	14
1.4.3	Dopant Diffusion . . . . .	15
1.5	Aims and Chapter Summaries . . . . .	16
<b>2</b>	<b>Theory Background</b>	<b>19</b>
2.1	The Many Body Problem . . . . .	19
2.1.1	Born-Oppenheimer Approximation . . . . .	20
2.1.2	Variational Principle . . . . .	22
2.1.3	Hartree's Method . . . . .	23
2.1.4	Hartree-Fock Theory . . . . .	25
2.2	Density Functional Theory . . . . .	26
2.2.1	Kohn-Sham Equations . . . . .	28
2.2.2	Exchange and Correlation Energies . . . . .	29
2.2.3	Pseudopotentials . . . . .	30
2.2.4	Choice of Boundary Conditions . . . . .	32
2.3	Chapter Summary . . . . .	33
<b>3</b>	<b>Theoretical Methods</b>	<b>34</b>
3.1	AIMPRO . . . . .	34
3.1.1	Supercell AIMPRO . . . . .	34
3.1.2	Cluster AIMPRO . . . . .	37

3.2	Cluster and Supercell Comparison . . . . .	38
3.2.1	Introduction . . . . .	38
3.2.2	Results . . . . .	40
3.3	Calculation of Observables . . . . .	42
3.3.1	Defect Structure . . . . .	42
3.3.2	Formation Energies . . . . .	44
3.3.3	Binding Energies . . . . .	46
3.3.4	Energy Levels . . . . .	47
3.3.5	Diffusion Barriers . . . . .	50
3.4	Calculation Parameters . . . . .	52
3.5	Chapter Summary . . . . .	54
<b>4</b>	<b>Experimental Methods</b>	<b>56</b>
4.1	Introduction . . . . .	56
4.2	Deep Level Transient Spectroscopy . . . . .	56
4.2.1	Deep Levels . . . . .	57
4.2.2	The Junction . . . . .	59
4.2.3	Capture and Emission . . . . .	60
4.2.4	Vacancy Clusters Observed in Electron-Irradiated Silicon . . . . .	63
4.3	Positron Annihilation Spectroscopy . . . . .	65
4.3.1	Experimental Set-Up . . . . .	65

4.3.2	Annihilation . . . . .	66
4.3.3	Vacancy Clustering in ZnO . . . . .	68
4.4	Secondary Ion Mass Spectroscopy . . . . .	69
4.4.1	Basic Principles . . . . .	70
4.4.2	Primary Ion-Sample Interactions . . . . .	71
4.4.3	Nitrogen Incorporation in GaNAs . . . . .	72
4.5	Spreading Resistance Profiling . . . . .	73
4.5.1	Evolution of Boron Interstitial Clusters in Silicon . . . . .	73
4.6	Transmission Electron Microscopy . . . . .	74
4.6.1	Controlling the Electron Beam . . . . .	74
4.6.2	Sample Restrictions . . . . .	75
4.6.3	Real-Time Imaging of Gold Nanowire Evolution . . . . .	76
4.7	Scanning Tunnelling Microscopy . . . . .	78
4.7.1	Self Assembly of Ordered Bi Patterns on InAs . . . . .	78
4.8	Summary . . . . .	79
<b>5</b>	<b>Intrinsic Defects in Germanium</b>	<b>80</b>
5.1	Introduction . . . . .	80
5.2	Modelling Method . . . . .	81
5.3	Divacancy Annealing . . . . .	81
5.3.1	Results . . . . .	83

5.3.2	Discussion . . . . .	88
5.4	Vacancy Clustering . . . . .	90
5.4.1	Results . . . . .	91
5.4.2	Discussion . . . . .	93
5.5	Self Interstitial Diffusion . . . . .	95
5.5.1	Results . . . . .	95
5.5.2	Discussion . . . . .	97
5.6	Chapter Summary . . . . .	97
<b>6</b>	<b>Dopant-Related Defects</b>	<b>99</b>
6.1	Introduction . . . . .	99
6.2	Modelling Method . . . . .	100
6.3	Arsenic-Boron-Vacancy defects in Silicon . . . . .	100
6.3.1	Defect Structures . . . . .	101
6.3.2	Energy Levels . . . . .	104
6.3.3	Formation Energies . . . . .	105
6.3.4	Migration Energies . . . . .	105
6.3.5	Discussion . . . . .	107
6.4	Donor-Vacancy Clusters in Germanium . . . . .	109
6.4.1	Energy Levels . . . . .	111
6.4.2	Formation Energies . . . . .	112

6.4.3	Migration Energies . . . . .	112
6.4.4	Discussion . . . . .	113
6.5	Chapter Summary . . . . .	115
<b>7</b>	<b>Dopant Diffusion in Germanium</b>	<b>117</b>
7.1	Introduction . . . . .	117
7.2	Modelling Method . . . . .	118
7.3	Phosphorus Diffusion . . . . .	119
7.3.1	Vacancy Mediated Diffusion . . . . .	121
7.3.2	Interstitial Mediated Diffusion . . . . .	123
7.3.3	Correlated Exchange (CE) . . . . .	127
7.3.4	Discussion . . . . .	127
7.4	Boron Diffusion . . . . .	130
7.4.1	Interstitial Mediated Diffusion . . . . .	131
7.4.2	Vacancy Mediated Diffusion . . . . .	136
7.4.3	Correlated Exchange . . . . .	137
7.4.4	Discussion . . . . .	137
7.5	Chapter Summary . . . . .	140
	<b>Conclusion</b>	<b>142</b>

# List of Figures

1.1	Three possible configurations of an interstitial atom in a diamond structure crystal. . . . .	4
1.2	Schematic diagram of dislocation structures. . . . .	11
3.1	Diagram showing the relationship between formation energy and energy levels of a defect. . . . .	48
3.2	Schematic diagram of the marker method. . . . .	49
4.1	Diagram showing the band bending present at a $p^+n$ junction. . . . .	59
4.2	Schematic diagram illustrating the action of a filling pulse in majority carrier DLTS. . . . .	61
4.3	Schematic diagram illustrating the double boxcars measurement used in DLTS . . . . .	62
4.4	PAS results showing $V_{Zn}$ void evolution in ZnO with annealing time. . . . .	69
4.5	TEM images of void growth in Au nanowires . . . . .	77
5.1	Diagram depicting the shape of the diffusion barrier of the divacancy. . . . .	84
5.2	Divacancy band structure as calculated between the $\Gamma$ point and two $L$ points. . . . .	85

5.3	Diagram describing the two types of Jahn-Teller distortion of the divacancy. . . . .	88
5.4	Diagram showing the structure of clusters of up to 14 vacancies. . . . .	92
5.5	Graph of the formation energy and number of dangling bonds per vacancy for clusters of up to 14 vacancies. . . . .	93
5.6	Graph showing the calculated first and second acceptor states of clusters of up to ten vacancies. . . . .	94
5.7	Diagram describing the ‘short’ and ‘long’ diffusion steps of the $I_{110}$ defect. . . . .	96
6.1	Examined structures for the AsBV defect complex. . . . .	102
6.2	Diffusion path taken by AsV in silicon . . . . .	106
6.3	Diagram of the diffusion path taken by $As_2V$ in silicon. . . . .	107
6.4	Diagram of the diffusion barriers for the $P_2V$ defect. . . . .	114
7.1	Structures of the phosphorus interstitial complex. . . . .	124
7.2	Diagram describing the migration steps for the $P_{iX_2}$ structure of the phosphorus interstitial. . . . .	125
7.3	Migration barriers for the $P_i$ defect in the singly negative, neutral and singly positive charge states. . . . .	126
7.4	Diffusion barrier dependence on Fermi level position for phosphorus complexes as calculated using the formation energy and marker methods for energy levels. . . . .	129
7.5	Interstitial-mediated boron diffusion steps along the $\langle 110 \rangle$ chain. . . . .	133

7.6	Interstitial-mediated boron diffusion steps for the singly positively charged structure. . . . .	134
7.7	Diagrams showing the barriers for BI complex migration in the singly negative, neutral and singly positive charge states. . . . .	135
7.8	Diffusion barrier dependence on Fermi level position for boron complexes. . . . .	139

# List of Tables

3.1	Binding energies, migration barriers and energy levels of V and V <sub>2</sub> in Si. . . . .	41
5.1	Binding energy of V <sub>2</sub> in germanium with increasing separation. . . . .	86
5.2	Binding (E <sub>b</sub> ), migration (E <sub>m</sub> ) and symmetry constrained saddle point (E <sub>scsp</sub> ) energies, in eV, of the divacancy in germanium. . . . .	86
5.3	Inter-atomic distances for atoms surrounding the divacancy. . . . .	89
6.1	Relative energies of different AsBV structures. . . . .	103
6.2	Inter-atomic separation around the As <sub>x</sub> B <sub>y</sub> V defects in silicon. . . . .	103
6.3	Energy levels of As <sub>x</sub> B <sub>y</sub> V defects in silicon. . . . .	104
6.4	Formation energy of As <sub>x</sub> B <sub>y</sub> V defects in silicon. . . . .	105
6.5	Total diffusion barriers for As via the formation of AsV and As <sub>2</sub> V defects in silicon. . . . .	107
6.6	Energy levels of P <sub>x</sub> V <sub>y</sub> clusters in germanium. . . . .	111
6.7	Formation energies calculated of P <sub>x</sub> V <sub>y</sub> clusters in germanium. . . . .	112
7.1	Formation energies and energy levels of the PV defect. . . . .	122

7.2	Formation energies and energy levels of the $P_2V$ defect. . . . .	122
7.3	Formation energies and energy levels of the PI defect. . . . .	124
7.4	Total migration energies for the PV and PI defects. . . . .	127
7.5	Energy change upon separation of the $BI^-$ defect along a $\langle 110 \rangle$ chain.	132
7.6	Energy change upon separation of the $BV^-$ defect along a $\langle 110 \rangle$ chain.	137
7.7	Total diffusion energies in eV for the BV, BI and boron CE mechanisms	138