



Structure, electronic properties, and interactions of defects in epitaxial GaN layers

Phillip H. Weidlich

Forschungszentrum Jülich GmbH
Peter Grünberg Institute (PGI)
Microstructure Research (PGI-5)

Structure, electronic properties, and interactions of defects in epitaxial GaN layers

Phillip H. Weidlich

Schriften des Forschungszentrums Jülich
Reihe Information / Information

Band / Volume 34

ISSN 1866-1777

ISBN 978-3-89336-951-5

Contents

1. Introduction	7
I. Theoretical principles and experimental techniques	11
2. Theory of the scanning tunneling microscope	13
2.1. Fundamental theory	13
2.2. Theory of the band structure	19
3. Properties of wurtzite gallium nitride	23
4. Experimental techniques	27
4.1. Preparation of samples	27
4.2. Preparation of tips	29
4.3. Correction of nonlinear distortions in STM images	29
5. Experimental details	37
5.1. Experimental details of Part II	37
5.2. Experimental details of Part III and Part IV	38
II. Hidden surface states at GaN (10\bar{1}0) surfaces	39
6. Introduction	41
7. Initial experiment	43
7.1. Experimental results	43
7.2. Discussion of the tunneling spectra	44

8. Ab initio calculations	47
8.1. Calculation method	47
8.2. Surface states and dispersion	49
8.3. Decay of the DOS into the vacuum	50
9. Experimental identification of the surface state	55
9.1. Modified experiment	55
9.2. Experimental results and discussion	58
III. XSTM of v-shaped defects in gallium nitride	61
10. Introduction	63
11. Doping modulation in epitaxial gallium nitride	65
11.1. Features on large scale STM images	65
11.2. Characterization of the modulation	68
11.3. Discussion of the contrast	69
12. Evidence of deep traps	73
12.1. Scanning tunneling microscopy observations	73
12.2. Determination of the geometric structure	75
12.3. Scanning tunneling spectroscopy on v-shaped defects	78
12.4. Discussion of the electronic properties	79
13. Meandering of v-shaped defects	83
13.1. Experimental observations	83
13.2. Quantification of the meandering	85
13.3. Determination of the origin of the meandering	87
IV. Characterization of dislocations and their interactions	91
14. Introduction	93

15. Repulsive interactions of dislocations	95
15.1. Experimental observations	95
15.2. Distribution of the dislocations	98
15.3. Discussion	102
16. Analysis of dislocations	105
16.1. Determination of the intersection angle of the dislocation line	105
16.2. Simulation of the displacement field of a dislocation	112
17. Conclusion	115
Bibliography	117
List of Figures	131
Abbreviations	133
Symbols	135



**Information/Information
Band / Volume 34
ISBN 978-3-89336-951-5**

