



Interface Functionalization of Magnetic Oxide $\text{Fe}_3\text{O}_4/\text{SrTiO}_3$ Heterostructures

Mai Hussein Abdalla Hamed

Schlüsseltechnologien / Key Technologies

Band / Volume 231

ISBN 978-3-95806-535-2

Forschungszentrum Jülich GmbH
Peter Grünberg Institut (PGI)
Elektronische Eigenschaften (PGI-6)

Interface Functionalization of Magnetic Oxide $\text{Fe}_3\text{O}_4/\text{SrTiO}_3$ Heterostructures

Mai Hussein Abdalla Hamed

Schriften des Forschungszentrums Jülich
Reihe Schlüsseltechnologien / Key Technologies

Band / Volume 231

ISSN 1866-1807

ISBN 978-3-95806-535-2

Contents

1	Introduction	1
2	Theoretical background	5
2.1	Magnetite versus other iron oxides	5
2.1.1	The ferrimagnetic half-metal: Magnetite (Fe_3O_4)	6
2.1.2	The antiferromagnetic: Wüstite (Fe_{1-x}O)	8
2.1.3	The ferrimagnetic insulator: Maghemite ($\gamma\text{-Fe}_2\text{O}_3$)	9
2.1.4	The antiferromagnetic insulator: Hematite ($\alpha\text{-Fe}_2\text{O}_3$)	9
2.2	Oxide substrates	10
2.2.1	Strontium titanate (SrTiO_3)	10
2.2.2	Yttria-stabilized zirconia (YSZ)	10
2.2.3	Epitaxial growth of Fe_3O_4 on oxide substrates and formation of anti-phase boundaries	11
2.3	Fundamental aspect of physical chemistry	12
2.3.1	Ellingham diagram	12
2.3.2	SrTiO_3 surface terminations and Gibbs free energy	13
3	Experimental Methods	15
3.1	Pulsed laser deposition (PLD)	15
3.2	Characterization techniques	16
3.2.1	Atomic force microscopy (AFM)	17
3.2.2	X-ray diffraction (XRD) and reflectivity (XRR)	17
3.2.3	Vibrating sample magnetometer (VSM)	19
3.3	Synchrotron-based X-ray spectroscopy	20
3.3.1	Fermi's golden rule	20
3.3.2	Three-step model of photoemission	21
3.3.3	Information depth	22
3.3.4	Photoemission spectral features	24

3.3.5	Hard X-ray photoelectron spectroscopy (HAXPES)	26
3.3.6	X-ray absorption spectroscopy (XAS)	27
3.3.7	X-ray magnetic circular dichroism (XMCD)	27
4	Growth optimization of $\text{Fe}_3\text{O}_4/\text{SrTiO}_3$ heterostructures	31
4.1	PLD growth conditions	32
4.2	Surface morphology and structural characterization	32
4.2.1	Experimental details	32
4.2.2	AFM	33
4.2.3	XRR	34
4.2.4	XRD	35
4.2.5	Discussion	37
4.3	Chemical and magnetic structure	38
4.3.1	Experimental details	38
4.3.2	HAXPES	40
4.3.3	XAS and XMCD	40
4.4	Magnetic characterization	45
4.4.1	Experimental details	45
4.4.2	Saturation magnetization	46
4.4.3	Coercivity and remanent magnetization	48
4.4.4	Verwey transition	49
4.5	Growth-induced lattice strain versus magnetic easy axis?	51
4.5.1	Experimental details	51
4.5.2	Tensile strain (500 °C)	52
4.5.3	Compressive strain (350 °C)	54
4.5.4	Discussion	56
4.6	Conclusion	57
5	Tunable ferri-magnetic phases at $\text{Fe}_3\text{O}_4/\text{SrTiO}_3$ oxide interfaces	59
5.1	PLD growth conditions	60
5.2	Structural and magnetic characterization	60
5.2.1	Experimental details	60
5.2.2	Structural properties	60
5.2.3	Saturation magnetization	62
5.2.4	Verwey transition	62
5.3	Buried $\text{Fe}_3\text{O}_4/\text{SrTiO}_3$ interface	65
5.3.1	Experimental details	65
5.3.2	HAXPES	65
5.3.3	Angle-dependent HAXPES	67
5.4	Interface magnetic properties	67
5.4.1	Experimental details	67
5.4.2	XAS and XMCD	67
5.4.3	Spin and orbital moment: the sum rules	70
5.4.4	Interface magnetic thickness	72
5.5	Substrate-induced interface oxidation	75

5.6	Towards stable $\text{Fe}_3\text{O}_4/\text{SrTiO}_3$ interfaces via annealing	76
5.6.1	Surface morphology	76
5.6.2	Structural properties	77
5.6.3	Saturation magnetization	78
5.6.4	Verwey transition	78
5.6.5	HAXPES	79
5.7	Conclusion	80
6	Growth of Fe_3O_4 on "inert" YSZ oxide substrates	81
6.1	PLD growth conditions	82
6.2	Growth temperature: structural and magnetic characterization	82
6.2.1	Experimental details	82
6.2.2	Structural properties	82
6.2.3	Saturation magnetization	84
6.2.4	Verwey transition	84
6.2.5	Summary	84
6.3	Thickness dependent: HAXPES	86
6.3.1	Experimental details	86
6.3.2	HAXPES	86
6.3.3	Discussion	87
6.4	Substrate-assisted interface oxidation	87
6.5	Conclusion	88
7	Thermally induced magnetic phase transition of iron oxides	89
7.1	Introduction	89
7.2	Experimental setup	90
7.3	HAXPES fitting routine	91
7.4	Annealing of ultrathin iron oxide films in UHV and in oxygen	93
7.4.1	HAXPES	93
7.4.2	Discussion	95
7.5	Annealing of ultrathin and bulk-like iron oxide films in UHV	97
7.5.1	HAXPES	97
7.5.2	Relative iron-compositions	99
7.5.3	Discussion	99
7.6	Annealing of ultrathin iron oxides films on NSTO and YSZ substrates	101
7.6.1	HAXPES	101
7.6.2	Relative iron-compositions	103
7.6.3	Discussion	103
7.7	Thermodynamics analysis	105
7.7.1	The van 't Hoff analysis	105
7.7.2	Thermodynamics parameters with unity effective oxygen pressure	108
7.7.3	Thermodynamics parameters considering the effective oxygen pressure	108
7.7.4	The calculated effective oxygen pressure and the standard phase diagram: adjusted phase diagram	109

7.8 Conclusion	111
8 Conclusion and Outlook	113
Appendix	117
A.1 XRR simulation	117
A.2 Simulation of XMCD spectra	120
A.3 Optimization of magnetite's growth parameters: pressure, laser fluence and frequency	123
A.4 Nb:SrTiO ₃ surface preparation	126
List of Abbreviations	127
Bibliography	129

Schlüsseltechnologien / Key Technologies
Band / Volume 231
ISBN 978-3-95806-535-2