



# Magnetic Properties of Self-assembled Manganese Oxide and Iron Oxide Nanoparticles

## Spin Structure and Composition

Xiao Sun

Schlüsseltechnologien / Key Technologies  
Band / Volume 176  
ISBN 978-3-95806-345-7

Forschungszentrum Jülich GmbH  
Jülich Centre for Neutron Science (JCNS)  
Quantenmaterialien und kollektive Phänomene (JCNS-2 / PGI-4)

# **Magnetic Properties of Self-assembled Manganese Oxide and Iron Oxide Nanoparticles**

## Spin Structure and Composition

Xiao Sun

Schriften des Forschungszentrums Jülich  
Reihe Schlüsseltechnologien / Key Technologies

Band / Volume 176

---

ISSN 1866-1807

ISBN 978-3-95806-345-7

# Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
<b>2</b>	<b>Theoretical Background</b>	<b>4</b>
2.1	Basics of Magnetism . . . . .	4
2.1.1	Magnetic Moments . . . . .	4
2.1.2	Isolated Magnetic Moments . . . . .	5
2.1.3	Anisotropy . . . . .	6
2.1.4	Interactions . . . . .	7
2.1.5	Magnetic Order . . . . .	10
2.1.6	Magnetic Domains . . . . .	12
2.1.7	Exchange Bias . . . . .	13
2.2	Basics of Nanomagnetism . . . . .	14
2.2.1	Superparamagnetism . . . . .	17
2.2.2	Interacting Nanoparticles . . . . .	18
2.3	Self-assembly . . . . .	20
2.4	Scattering Theory . . . . .	21
2.4.1	Basics of Scattering . . . . .	21
2.4.2	Diffraction . . . . .	23
2.4.3	Polarization Analysis . . . . .	24
2.4.4	Small Angle Scattering . . . . .	27
<b>3</b>	<b>Monte Carlo Simulations</b>	<b>30</b>
3.1	Basics of Monte Carlo Simulations . . . . .	30
3.2	Physical Models . . . . .	31
3.3	Simulation Procedures . . . . .	32
<b>4</b>	<b>Experimental Methods and Instruments</b>	<b>34</b>
4.1	Magnetometry . . . . .	34
4.2	AC-Susceptibility . . . . .	37
4.3	Heat Capacity . . . . .	37
4.4	Torque Magnetometry . . . . .	38
4.5	X-ray Diffraction . . . . .	38
4.6	Neutron Diffraction . . . . .	39
4.7	(Grazing Incidence) Small Angle X-ray Scattering . . . . .	40
<b>5</b>	<b>Investigation of the Spin Structure of Manganese Oxide</b>	<b>42</b>
5.1	Introduction to Manganese Oxide . . . . .	42
5.2	Sample Preparation . . . . .	44
5.2.1	Synthesis of MnO Nanoparticles . . . . .	44
5.2.2	Annealing of Powder and Single crystal . . . . .	44
5.2.3	Annealing of Nanoparticles . . . . .	45
5.3	Structural Characterization . . . . .	46
5.4	Experimental Results . . . . .	50
5.4.1	As-prepared MnO Nanoparticles . . . . .	50
5.4.2	As-prepared MnO Bulk . . . . .	52
5.4.3	Annealed MnO . . . . .	61

---

5.5	Monte Carlo Simulations . . . . .	68
5.5.1	Spin Structure Visualization . . . . .	80
5.6	Summary . . . . .	93
<b>6</b>	<b>Magnetism of Iron Oxide Nanoparticle Superstructures</b>	<b>98</b>
6.1	Introduction to Iron Oxides . . . . .	98
6.1.1	Phases of Iron Oxide . . . . .	98
6.1.2	Iron Oxide Nanoparticles . . . . .	100
6.2	Current State of Research on Self-Assembly . . . . .	102
6.3	Sample Preparation . . . . .	104
6.3.1	Self-Assembly . . . . .	104
6.3.2	Sample Annealing . . . . .	110
6.4	Structural Characterizations . . . . .	112
6.5	Experimental Results . . . . .	114
6.6	Summary . . . . .	138
<b>7</b>	<b>Summary and Outlook</b>	<b>141</b>
<b>Appendix A Parameters used in MC simulations</b>		<b>143</b>
<b>Appendix B Convergence test with various Monte Carlo steps</b>		<b>144</b>
<b>Appendix C XRD patterns of MnO powder after various treatments</b>		<b>145</b>
<b>Appendix D Magnetometry results of MnO</b>		<b>146</b>
<b>Appendix E Polarized Neutron diffraction</b>		<b>148</b>
<b>Appendix F Monte Carlo Simulations</b>		<b>150</b>
<b>Appendix G Spin Visualizations</b>		<b>154</b>
<b>Appendix H SEM Images of Iron Oxide NPs</b>		<b>160</b>
<b>Appendix I Magnetization curves of Iron Oxide NPs</b>		<b>162</b>
<b>8</b>	<b>References</b>	<b>167</b>

Schlüsseltechnologien / Key Technologies  
Band / Volume 176  
ISBN 978-3-95806-345-7