

I Table of contents

I	Table of contents	i
II	Abstract	iv
III	Preface	xi
IV	List of contributing publications	xii
V	List of figures	xiv
VI	List of tables	xvii
VII	Symbols and abbreviations	xviii
VIII	Acknowledgements	xxiv
1	Introduction	1
1.1	Motivation	3
1.2	Goals	3
1.3	Structure of the thesis	5
2	Theoretical methods	7
2.1	Density functional theory	7
2.2	<i>Ab initio</i> calculation methods	8
3	Experimental methods	12
3.1	Thin film growth	12
3.1.1	Combinatorial DC magnetron sputtering	12
3.1.2	Experimental setup	14
3.2	Thin film characterization	17

3.2.1	XRD and EBSD analysis of the structure and crystallographic texture	18
3.2.2	EDX and WDX analysis of the chemical composition.....	21
3.2.3	Nanoindentation measurements of the local mechanical properties....	22
4	Results and discussion	28
4.1	Fe-Mn-C alloys	28
4.1.1	Chemical composition.....	28
4.1.2	Structure and crystallographic texture.....	32
4.1.3	Elastic properties	37
4.1.4	Electronic structure	40
4.2	Fe-Mn-C-Al alloys.....	41
4.2.1	Chemical composition.....	41
4.2.2	Elastic and plastic properties.....	43
4.2.3	Pile-up behavior	46
4.3	Fe-Mn-Al alloys	48
4.3.1	<i>Ab initio</i> calculations of the elastic properties	48
4.3.2	Experimentally determined elastic properties	50
4.3.3	Structure, crystallographic texture and phase formation	53
4.4	Fe-Mn-X (X = Cr, Co, Ni, Cu) alloys	58
4.4.1	<i>Ab initio</i> calculations of the elastic properties	58
4.4.2	Experimentally determined elastic properties	66
5	Conclusions	73

I Table of contents	iii
6 Future work	79
IX References.....	xxvi