Chapter 1

Introduction

The electron was discovered in 1897 by J.J. Thomson as an elementary particle embodying a finite amount of charge. The charge property makes a (moving) electron in free space interact with electromagnetic fields via the Coulomb and Lorentz forces and enables metals and semiconductors to carry an electrical current.

The observation of the Zeeman effect in 1896 and fine structure anomalies in the line spectra of atoms led to the suggestion that the electron also has a spin. The electron spin provides another degree of freedom for the electron to interact with a magnetic field. The most direct experimental proof of the existence and quantized nature of the electron spin ($S_z = 1/2$) was obtained by Stern and Gerlach in 1922. The concept of spin for electrons was introduced in 1925 by Uhlenbeck and Goudsmit [7]. They suggested that the electron spin acts like an intrinsic angular momentum (S) with a magnetic moment associated to it.

The quantization of the spin of a free electron imposes that, whenever it is measured, it can have only one of two possible values: spin-up and spin-down.

Using the spin of the electron besides its charge, creates a remarkable new generation of microelectronic devices. This field of research has been labelled with the term spintronics and has seen a rapid growth over the past few years. The most well known examples of spin dependent electron transport phenomena is the giant magnetoresistance (GMR) effect in metallic multilayers [8–12] and tunneling magnetoresistance (TMR) of magnetic tunnel junctions [13, 14].

Heterojunctions between a semiconductor and a ferromagnetic metal have attracted attention in the context of spintronics. The study of magnetism in thin films and low-dimensional systems is one of the most prospering areas of modern solid state physics. As a matter of fact the magnetic properties of these structures differ from those of the constituent bulk materials in many different ways. The research in this field revealed some new interesting phenomena like the anti-ferromagnetic coupling in magnetic / non-magnetic multilayered structures, which leads to the giant magnetoresistance effect.

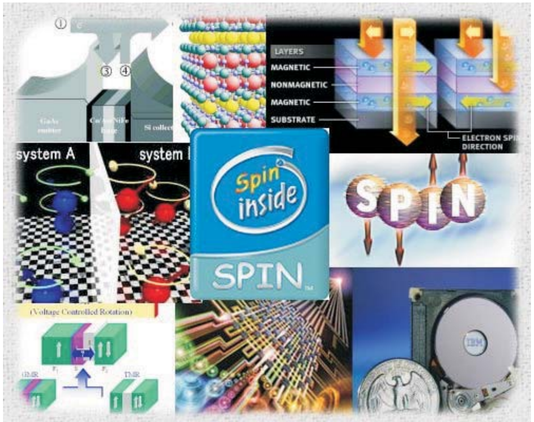

Fig. 1.1: Electronics with spin: current research and future possibility. Figure is adapted from "http://www. spintronics.inha.ac.kr"

Metal-semiconductor heterojunctions hold great promise for fabrication of spintronics devices, because of the possibility to inject a spin current from a ferromagnetic metal into a semiconductor. For computational materials science, this poses the challenge of designing materials that are suitable to inject a spin-polarized current into a semiconductor.

The spin-injection efficiency into semiconductors could be produced either by using a diluted magnetic semiconductor or, by fabrication of magnetic metal films on a semiconductor. Epitaxial growth of transition metal monosilicide ferromagnetic films on a Si substrate can be used as a source of spinpolarized carrier injection to semiconductors which can be applied for spintronics devices. The requirements for such a material are i) it should show (preferably ferro-)magnetic ordering above room temperature, ii) have a high spin polarization of carriers at the Fermi level, and iii) be structurally compatible with silicon. Here, we want to put forward magnetic intermetallic compounds grown epitaxially on Si as promising candidate materials. Epitaxial Mn-silicide compounds are promising candidates for the components of microelectronic and spintronic devices applications. The high magnetization of Mn and compatible lattice match of Mn and Si make it suitable to create a magnetic interface of Mn (-silicide) on a Si substrate. Most of the experiments about Mn deposition on Si report about formation of a Mn-silicide compound. In 1985 the epitaxial growth of (001)$MnSi_{1.7}$ / Si(001) and (1$\bar{1}$0)$MnSi_{1.7}$ / Si(111) was reported by analysis of electron diffraction patterns [15] and recently, flat islands of MnSi and three-dimensional islands with Mn_5Si_3 structure on Si(001) [16] as well as (relatively) big islands consisting of MnSi were observed on Si(111) [17]. Moreover, among the known bulk phases of Mn silicides, Mn_3Si in the $D0_3$ structure appears to be compatible with pseudomorphic thin film growth on Si surfaces

The epitaxial growth of a film of Mn-silicide on Si(111) with the help of a Bi surfactant layer [18–21] has been reported. The nearly closed film at higher coverage (more than 5 ML) was observed with the scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) [22].

1.1 Goal and Outline

The aims of this thesis are to investigate the structure and magnetic interactions in multilayer systems and how these affect their magnetic properties.

In an attempt of 'computational materials design', we investigate the stability and magnetic properties of Mn on the Si substrate in both Si(001) and Si(111) orientations.

We have studied Mn incorporation at Si(001) and Si(111) surfaces within density functional theory using the full-potential augmented plane wave plus local orbital method (FP-LAPW+lo). The basis set of this method (i.e. choosing angular momentum eigen functions around atomic positions and plane waves in the interstitial region), make it a suitable tool to study the behavior of transition metals with localized d orbitals. The detailed features of the method and computer package which is used in this thesis are described in **Chapter 2**.

To understand the mechanisms of the nanoscale structures such as thin films and to contrast the different properties of the film with its constituents in intermetallic multilayers, one needs to have good information about the bulk phases. In **Chapter 3**, bulk properties of plausible compounds which could be grown on Si surfaces are studied. Structure and thermodynamic stability as well as electronic and magnetic properties of bulk crystals are the quantities to compare with epitaxial films grown on the surface.

One requirement needed to simulate the growth on surfaces, the morphology of films and the properties of interfaces and surfaces is a sufficient knowledge about the surface on which the growth take place. In **Chapter 4** the morphology of Si(001) and Si(111) surfaces as well as the surface reconstructions for Si(001) are discussed.

The initial step which one needs to know the starting point for simulating the growth process is finding stable adsorption sites on the surface and surface diffusion. We show in **Chapter 5** that the sub-surface second layer is the most stable adsorption site for Mn with an adsorption energy of 3.8 eV. Besides, we calculated the adsortion energy at the substitutional site and also the adsorption on a surface defect site. In this chapter, we also estimate the energy barrier for diffusion on the surface and for penetration to the sub-surface site.

The morphology and stability of films on Si surfaces, magnetic properties of interfaces and surfaces are presented in **Chapter 6** and in the first part of **Chapter 7**. The stability of Mn_xSi_y films on Si has been investigated for various stoichiometries and atomic structures of the films. We propose the formation of a film with with Mn-monosilicide in the cesium chloride (B2)(001) structure on Si(001). Due to suitable interface with Si(111) the natural phase (B20) of MnSi stabilizes on this substrate. Additionally, the formation energy of these films versus coverage is also discussed.

Finally in the second part of **Chapter 7**, we focus on the film stability against island formation and we calculate the energy associated with island formation of a certain size as a function of film thickness and coverage.