Chapter 1

Introduction

1.1 Overview

The spatial dimensions of semiconductor devices have been shrinking since the invention of the transistor by Bardeen, Brattain, and Schockley in 1947 [1]. The motivation for the reduction of device size is manyfold: One the one hand the efforts are aimed at a higher area density and therefore an increased integration of circuits. On the other hand smaller devices result in higher speeds as well as lower power consumption: Free carriers can travel smaller distances in a shorter time, and it takes less carriers to switch a device due to the reduced capacitance.

While one could build the first transistor by handcraft (see fig. 1.1), the device dimensions on a commercially available microprocessor (at the time of writing) are on the order of $0.13\mu m$ (see for example ref. [3]). Laboratory pilot devices for the next generation's scale amounts to 90nm (i. e. on the order of 400 atoms in one dimension) with smallest separation amounting to only 5 atomic layers [4]. At this moment, we are thus witnessing the transition from micro- to nanoelectronics. Vital to this development is the understanding of structure and electronic properties on the atomic scale. It has also been recognized that further reduction will increase the importance of quantum mechanical effects, which can be corruptive for the conventional device concepts, yet at the same time promising for new concepts [5].

Simultaneously with the emerging field of nanostructures, the invention of Scanning Tunneling Microscopy (STM) by Binnig and Rohrer [7] was a major breakthrough that won them the noble prize in 1986. STM is sensitive to the electronic properties of a conducting surface down to the atomic scale. Maybe the biggest advantage of this technique is, that it measures local properties in *real-space*, i. e. as a function of lateral displacement. This opens the possibility of studying individual, non-periodic features on the atomic scale. It is therefore an



Figure 1.1: The first transistor developed by John Bardeen, Walter Brattain and William Schockley at Bell Labs. It was a pnp point-contact germanium transistor operated as a speech amplifier with a power gain of 18 on December 23, 1947. For this work, Bardeen, Brattain, and Schockley were awarded the Noble prize in 1956. Image courtesy of Lucent Technologies [2].

ideal substitution for methods based on diffraction that average over some sample area or volume and measure physical properties in *reciprocal space*, i. e. as a function of spatial frequency.

A recent example, where the method of STM meets the field of computing and logic devices, was given by Heinrich and coworkers [6] (see fig. 1.2). By arranging individual CO molecules on a single crystal surface with the tip of an STM, they succeeded in building logic gates. The operation of these devices is based on the selective diffusion of the molecules. The device is build, triggered and read-out with the STM. The lateral size of these units is only of the order of several nm. Although such an approach will be of no practical use for some time to come (if ever), this work demonstrates the capabilities of the STM as a research tool and that the reduction of device size has a long way to continue before hitting fundamental limits from physical laws.

In this thesis, we have applied STM to study the atomic-scale structure and electronic properties of a prototypic metal-semiconductor contact. Metal-semiconductor contacts (MS contacts) are usually rectifying, a property which has been known for more than a century [8]. But it was not before 1938 until Schottky [9] and Mott [10] independently developed a first model for that behavior: The metal layer creates a potential barrier for majority charge carriers on the semiconductor side. The barrier increases or decreases depending on the applied bias voltage,



Figure 1.2: Two-input sorter. (A) Model of the sorter, which computes the logic AND and logic OR of the two inputs. The sorter consists of Co molecules individually arranged with the STM tip on the (111) surface of a Cu single crystal. (B to D) Succession of STM images (9 nm by 9 nm) I = 50pA; V = 10mV. Starting from the initial setup (B), input X was triggered by manually moving the top CO molecule, which propagated a cascade to the OR output (C). Input Y was subsequently triggered, which propagated a cascade to the AND output, as shown in (D). The sorter also operated correctly when input Y was triggered (not shown). Taken from ref. [6].

which leads to the rectifying properties. Schottky and Mott also gave an explanation for the mechanism of the formation of that barrier and came up with a first law determining the height of the barrier for different combinations of metal and semiconductor, the "Schottky-Mott Rule". Since then the terms metal-semiconductor contacts and Schottky contacts have been used synonymously.

Soon after the pioneering work by Schottky and Mott [9, 10], it became clear that the Schottky-Mott Rule is inadequate in predicting the observed barrier heights and that additional mechanism have to be invoked to account for the deviations. Since then, the physics of MS contacts have been a controversial issue [8, 11, 12, 13]. None the less successful in application, Schottky contacts are the core of modern microelectronics. The standard switching device in highly-integrated cir-

cuits is the CMOS [11], which uses the property of modulating the carrier density in the semiconductor under a metal gate and an insulating oxide layer. As integration of microelectronic circuits increases and devices scale down in size, the need emerges for understanding and characterizing MS interfaces on an atomic scale.

Recently, much research is carried out on using the spin of a carrier to transport information or switch in electronics, the so called "Spintronics" [14]. In order to manipulate spin, one has first to prepare a set of carriers with a pure spin state. A promising approach is a Schottky contact with a ferromagnetic metal. The carriers injected over the Schottky barrier into the semiconductor show a partial polarization of their spin, the device thus acts as a "spin injector" [15, 16]. This topic gave a new incentive in exploring Schottky physics, now with an emphasis on ferromagnetic overlayers.

1.2 The process

¹From the invention of the STM until now, this technique has undergone a huge development from simply "imaging" a surface: Now many related spectroscopic techniques are applied, such as current-voltage spectroscopy, workfunction measurements, tunneling-induced luminescence, surface photovoltage and many more. These spectroscopic techniques have increased the demands on data collecting and evaluation considerably. In the course of this thesis, some of these spectroscopic techniques were established in the research group of Dr. Wenderoth and Prof. Ulbrich, where this Ph. D. project was carried through. At the start of the project, the STM hardware (STM head and ultra high vacuum chamber), the measurement modes of atomically-resolved constant current imaging and the preparation of cross-sectional samples of GaAs and related III-V semiconductors were already well-established [17, 18]. However, tunneling spectroscopy was available only on a very rudimentary level. Many improvements on the setup had to be accomplished. Completely redesigned custom-made STM electronics were commissioned, which resulted in greatly increased sampling frequency, electronic stability, reduced noise level and reliability. Completely new STM control software code was written in object-oriented C++ programming language with graphical user interface. What makes this system stand out against commercially available STM electronics is a greatly enhanced adaptability of the system softwareelectronics to new measurement modes. Another big improvement had to be done in terms of tip preparation. The demands of spatially-resolved tunneling spectroscopy on semiconductors for the tunneling tips are high: Typical spectroscopic measurements last on the order of hours, in which the tip has to remain stable

¹Many coworkers and fellow students have contributed to the achievements and technical improvements who the author wishes to acknowledge. Please see the Danksagung.

1. Introduction

and sharp even when varying an external parameter (spectroscopy) over a large range. For achieving this, one of the crucial improvements was commissioning a dedicated tip preparation and load lock chamber in which the complete process of cleaning and sharpening the tips can now be done immediately before the measurement and without breaking the vacuum. Finally, the data analysis software had to be adapted to cope with the vast amount of spectroscopic data.

The preparation of cross-sectional samples of metal-semiconductor contacts was greatly improved by using a new-commissioned UHV chamber for metal molecular beam epitaxy [19, 20]. By use of electron beam evaporators, the back-ground pressure during evaporation and the pureness of the evaporated metal was greatly enhanced compared to the epitaxy by resistance heating already available in the group.

A final remark: The overview and big picture are surely important for the motivation and funding on a longer time scale, i.e. the lifetime of a Ph. D. project and longer. However, although this thesis is dealing with a material system important for technology, it is not about building devices. In fact, the direct applicability of the findings of this thesis in technology is very limited. To the author's experience the big picture rarely pops up, when bogged down in every day lab routine. Asking a fairly simple question to a prototypic sample system which can only be answered using quite elaborate experimental techniques was the driving force. So in the end, what carries one through the length of a project, is a mix of curiosity as well as competition.

1.3 The outline

In chapters 2 and 3 we give a brief introduction to the method of Scanning Tunneling Microscopy and Spectroscopy as well as to the structural and electronic properties of GaAs(110) surfaces, which is the reference system on which the Schottky contacts investigated in this work are based. Chapter 4 describes the experimental setup and methods used in this thesis. This includes the STM hardware, electronics, and software as well as the tip and sample preparation.

In chapter 5 we will present the basics of metal-semiconductor contacts and the mechanisms of Fermi level pinning (FLP). Having to choose from the vast amount on information available on this much-elaborated topic, this chapter is restricted to the bare necessities for facilitating the discussion of the results later on.

After this, chapters 6 and 7 give the results obtained with STM on MS contacts in cross-sectional configuration. Chapter 6 focusses on the structural characterization of the interface and the mechanisms of Fermi level pinning as visible in tunneling spectroscopy. Chapter 7 deals with the imaging of the barrier potential