Electron transport through single gold atoms and hydrogen molecules switching on the atomic scale
Trouwborst, Marius Leendert

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2009

Link to publication in University of Groningen/UMCG research database

Citation for published version (APA):

Copyright
Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

Take-down policy
If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): http://www.rug.nl/research/portal. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.
Summary

The research field of nanotechnology deals with structures below 100 nanometer (1 nanometer is $10^{-9}$ meter). It is expected that this technology will strongly develop in the next years. The ultimate question is whether one can control the process on the atomic scale, and use this for applications. Possibly, one could even make faster computer chips in the future consisting of molecules as the functional building blocks. At this moment, it is not yet clear if this will happen, more research is needed of the interactions on the atomic scale.

This thesis describes experimental research on electron transport through single atoms and molecules. This is possible by using a so called mechanically controllable break junction. Such a junction consists of a (golden) wire, which is fabricated on top of a flexible substrate (as shown on the cover page of this thesis). This wire can be stretched by bending the substrate and, with further stretching, the wire will break near the middle of the substrate. The interesting thing is that for metals like gold, the wire will become thinner and thinner upon stretching (like chewing gum). Just before rupture, the minimum diameter of the wire is only a single gold atom. After breaking, one has created 2 atomically sharp electrodes. By now bending back and forth the substrate, one can control the distance between the electrodes with a very high precision (with a precision in the order of picometers, or $10^{-12}$ meter). With this system, one can investigate the electronic and mechanical properties on atoms and molecules on the atomic scale.

First of all, it is crucial to know the precise distance between the electrodes. Therefore, one has to know the ratio between the bending of the substrate, and the change in electrode distance. This is not trivial. We show in chapter 3 that this depends on the exact geometry of the system. Luckily, there are experimental methods to measure the electrode distance, and to calibrate the break junctions. In this thesis, three independent methods are used. An example is to measure the tunnel current. At electrode distances smaller than 1 nm, electrons can quantum mechanically tunnel from one electrode to the other. This current can
be measured directly, and has an exponential dependence with distance. This way, one can accurately determine the electrode distance.

It is not possible to set the electrode distance at any given value. Instead, the two wires ”jump” into contact at small electrode separations. This occurs at typical distances of 1.5 Ångstrom (1 Ångstrom = 10^{-10} m), and is investigated in chapter 4. This effect is a direct consequence of the binding energy of the opposing atoms of the two wires, which results in an attractive force between the wires. At small separations, this force is so strong that the wires are pulled towards each other, and even jumping into making contact. Subsequently, when pulling the wire, the wire will first be stretched before it breaks. Till thus far, it was not possible to model this process. The reason is plastic deformation. Every time the wire is broken, the atoms arrange themselves in a somewhat different configuration. We have found a method to eliminate this plastic deformation. This method is based on multiple times breaking and making of the wire. When this is done in a controllable way, then this ”training” of the wire leads to an ordering of the gold atoms. For the new formed wires the breaking process can be modeled with high precision, with only the elasticity of the electrodes as fit parameter (between 5 and 32 N/m). This gives new insight in the electron transport on the atomic scale.

The process described above results in atomically sharp electrodes. With this system, one can ”catch” a molecule for investigating its electrical properties. In this thesis, measurements are described on hydrogen molecules. Hydrogen, as a simple molecule, is an ideal system for studying the interactions on the atomic scale. An example of such interactions is the molecular vibrations of the hydrogen molecule. By measuring the electron transport through a hydrogen molecule, one can deduce the conductance of a single molecule. Subsequently, when the energy of the electrons is large enough (above a certain threshold voltage), the molecule can use the electron energy for the excitation of a molecular vibration. The molecule then vibrates in between the electrodes (comparable to a guitar string). However, the influence of these excitations on the conductance properties of the molecule is not yet completely understood. For example, these vibrations often result in a sudden changes of the current through the contact. This phenomenon is investigated and its results are reported in chapter 5. For this study, the molecules are vibrationally excited by a voltage pulse, after which the current response has been measured. This gave some unexpected results. Namely, the lifetime of a molecular vibration is expected to be small (smaller than 1 ns). Instead, we have observed response times as long as 200 ms. Apparently, a
large amount of energy has been put into the system, which needs a long time to flow away into the electrodes. Although it is difficult to draw a detailed conclusion, our observations are consistent with a phase change of the hydrogen. It is possible that the excitations of the molecules result in a strong heating of the molecules (including the molecules near the contact). This could result in a phase transition, for example from the solid phase to a liquid phase. Such heating effect by molecular vibrations has been theoretically predicted, but has never been shown experimentally. Another explanation could be the weak coupling between the molecules and the gold atoms. This could result in a long time scale, for the molecules to cool down.

The effect described above can even be used for an electronic switch (as described in chapter 6). With the help of small voltage pulses (as small as 2 mV), one can switch the system between two different conductance values. These voltage pulses are then added to a DC voltage, which is set equal to the vibration energy of the molecule. Also here, it is found difficult to give a precise description of the effect. However, it is clear that a heating effect plays a crucial role. It is possible to explain the results by a phase change depending on the exact molecular temperature. This could explain the energy difference between the different transitions (solid to liquid and vice versa). The results presented in chapters 5, 6 and 7 show that the vibration spectra of even simple molecules as hydrogen are not yet understood, and give interesting physics. Without any doubt this will result in new insights in the future.

All measurements described above are done with a break junction, where one breaks a gold wire with the help of a mechanical system. In the last chapter, we describe another method to create electrodes for molecular electronics. When a large current density is forced through a wire, the atoms in the wire will be pushed out their equilibrium position (at typical current densities of $10^8$ A/cm$^2$). This process is called electromigration, and can result in breaking of the wire. After breaking, one ends up with two electrodes, separated by only a few ångstroms. The main advantage of this system is that it is relatively easy to fabricate a large number of electrodes, which can be used for molecular electronics. We have studied this method, as described in chapter 8. The main conclusion is that electromigration only occurs at a minimum local temperature (around 400 Kelvin). This threshold temperature increases the mobility of the atoms, and has one important consequence. For using electromigration induced contacts for molecular electronics, methods have to be used to minimize the local temperature
during breaking.