Electrical Single Molecule Investigations by Means of Mechanical Break Junctions

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Abstract:

The mechanically controllable break junction (MCBJ) technique was employed to investigate the conductance of single molecules. Octanedithiols have been extensively investigated in previous work and were measured as a check of our techniques and equipment. Dendrimer molecules with a ferrocene core (CSA-FcGluOH) were measured using these techniques for the first time. Artifacts in the measurements resulting from our lithographically prepared samples hindered our ability to make accurate and reliable measurements. However, extensive studies of the MCBJ and measurement tool behaviors were carried out to improve future work.

Introduction:

As the size of silicone-based electronic components reaches its limit, investigations of alternative electronics technologies have become increasingly vital. One promising area is the field of molecular electronics. A crucial step towards realizing these goals is the characterization of a variety of molecules and their typical conductance values, reported in terms of the conductance quanta, G_0, of a single atom. Our chosen method for this process was the mechanically controllable break junction (MCBJ) technique. This employs a piezo to control the position of a pushrod, which then bends the flexible substrate upon which the junction lies. The contacts are separated with an aspect ratio in relation to the pushrod position on the order of 1:200000. This creates an incredibly stable junction because small vertical variations will not greatly influence the gap size. The MCBJ method was employed to investigate bare gold electrodes as well as 1,8-octanedithiol test molecules, which have been extensively investigated in previous work. The ultimate objective was to carry out the first investigations of a set of dendrimer molecules containing a ferrocene core.

Experimental Procedure:

Because of the variations in the single molecule contact geometries in the measurements, a statistical investigation was required [1]. This necessitated the taking of a large number of measurements. Such measurements involve opening the junction slowly with an applied voltage bias while recording current and voltage readings. The conductance values for single atom conductance and single molecule conductance are seen in these measurements as plateaus in the conductance vs. time plots as the junction is separated. An example can be seen in Figure 1, which is a plot from a nanowire sample with 1,8-octanedithiol molecules. The single atom conductance plateau can be seen at 10^{-6} amps, while the single molecule conductance plateau can be seen at 10^{-10} amps.

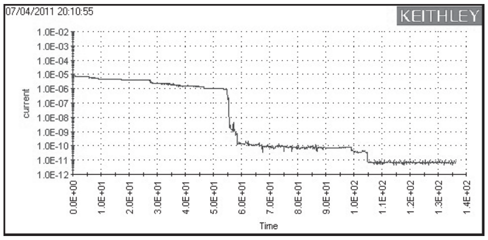

Figure 1: Current (amps) vs. time (seconds) curve for junction opening with 1,8-octanedithiol on nanowire. Voltage is 13 mV, pushrod velocity is 3 µm/sec.

After at least 100 such measurements are carried out with a given sample, the conductance values can be plotted in a histogram. The plateaus appear as peaks in the histogram corresponding to the various stable values observed throughout the breaking of the junction. A strong single atom peak should always be observed (along with less pronounced two and three atom peaks). Lower conductance peaks should then correspond to the typical conductance values of the molecules under investigation. The variation in these values corresponds to geometric and contact fluctuations as well as different possible molecular conformations across the junction.

Results and Conclusions:

Measurements were carried out with both macrowire (0.1 mm diameter gold wire glued to a spring steel substrate) and nanowire (lithographically fabricated gold on a spring steel substrate) samples. A histogram of the results from the macrowire samples with no molecules is shown in Figure 2 along with the histogram for the nanowire samples with no molecules. The artifacts observed in the nanowire histogram are not present in the macrowire data. The inset shows the high conductance region with single and multi-atom peaks, providing confirmation of the quality of our equipment and methods. Note how the peaks are more pronounced in the macrowire histogram. These results indicate that, while the nanowire samples should be more stable, macrowire samples can still provide more reliable results.

Figure 3 shows the histogram for the nanowire samples with 1,8-octanedithiol molecules. The artifacts in the histogram make the results less obvious, but a clear peak can still be seen around $10^{-4}G_0$, a similar result to previous work. Results in the literature can vary over a wide range, however, due to different electrode and apparatus designs. One previously published paper indicates a conductance between $10^{-4}G_0$ and $3*10^{-4}G_0$ [2].

Figure 4 shows histograms from five different nanowire samples with CSA-FcGluOH molecules. Note that there are no significant peaks found in all five histograms. This may be partially due to the large effect of the artifacts obscuring the results. However, since these molecules have not been measured before, it is possible that the conductance lies below our working range or, due to the increased length and complexity of these molecules compared to others commonly investigated, there may not be such well defined peaks to be found.

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References:

[1] Lörtscher, E. et al; "Statistical Approach to Investigating Transport Through Single Molecules"; Physical Review Letters, 98, 176807 (2007).

[2] Kim, Y. et al.; "Characteristics of Amine-Ended and Thiol-Ended Alkane Single-Molecule Junctions Revealed by Inelastic Electron Tunneling Spectroscopy"; ACS Nano, 5 (5), 4104-4111 (2011).

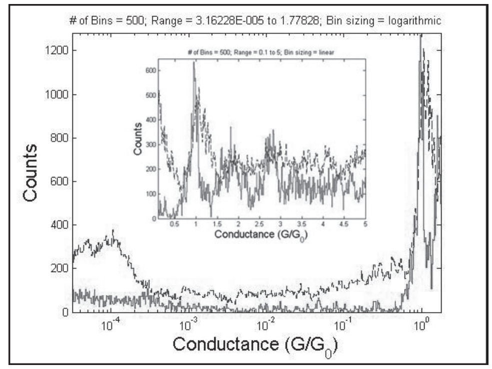

Figure 2: Histograms for both macrowire (solid) and nanowire (dashed) data with no molecules. 132 and 180 curves, respectively. Macrowire histogram scaled to match nanowire. Inset: High conductance region showing the atomic conductance peaks.

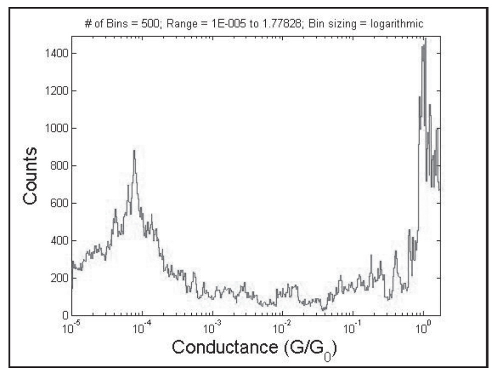

Figure 3: Histogram of data for 1,8-octanedithiol molecules measured with nanowire samples. 90 curves.

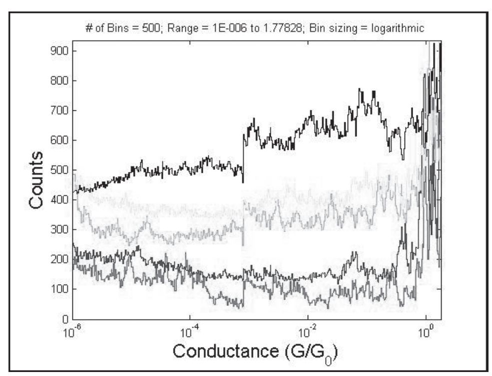

Figure 4: Histogram of data from four different samples of CSA-FcGluOH molecules measured with nanowire samples. 290 curves total (50-60 each). The histograms are shifted vertically to separate them.