

# The high-bias stability of monatomic chains

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## Abstract

For the metals Au, Pt and Ir it is possible to form freely suspended monatomic chains between bulk electrodes. The atomic chains sustain very large current densities, but finally fail at high bias. We investigate the breaking mechanism, that involves current-induced heating of the atomic wires and electromigration forces. We find good agreement of the observations for Au based on models due to Todorov and co-workers. The high-bias breaking of atomic chains for Pt can also be described by the models, although here the parameters have not been obtained independently. In the limit of long chains the breaking voltage decreases inversely proportional to the length.

## 1. Introduction

As the down-scaling of electronic components is advancing at an impressive rate, the general interest in dissipation and thermal transport at comparable scales is increasing. Technical applications using these small scale devices will have higher and higher densities of components, making heat generation one of the biggest problems to overcome. We therefore need to develop a better fundamental understanding of the properties of matter at small size scales. A recent review [1] on thermal transport at the nanoscale shows how fast this field has been growing during the last few years. It also shows that at scales of the order of several nanometres the quantum behaviour of matter starts to have a major impact on the thermal behaviour of the sample. As an example, Yao *et al* [2] have shown that the current through a single-wall carbon nanotube is saturating as the voltage reaches values of several volts, a behaviour which is not expected from a simple down-scaling of classical effects.

Here we study the thermal behaviour of metals at the smallest length-scales, below 1 nm. A review of results in this field has recently appeared [3]. In recent experiments it was shown that some metals have the property of spontaneously forming monatomic chains just before rupture [4, 5]. Although atomic chains are intrinsically metastable, experiments at high bias voltages showed they have a surprising current-carrying

capacity [4], and current densities up to  $10^9$  A mm<sup>-2</sup> could be reached. Currently the lengths of these chains is limited to about seven atoms. A better understanding of dissipation and relaxation phenomena may lead the way to fabricate longer chains. With these monatomic chains being nearly ideal one-dimensional conductors, this would provide a means to further study the fundamental properties of conductors in one dimension.

In the experiments described below we probe the stability of many individual monatomic chains by looking at their rate of survival at high bias voltages. Although these nanowires due to their small size are ballistic, high bias results in a small probability for inelastic scattering of the electrons to phonons. Energy dissipation has been demonstrated to come into play when  $eV$  for the bias voltages applied is raised above the characteristic zone-boundary phonon energy [6]. Energy dissipation will take place on the scale of the electron–phonon scattering length (typically  $\gg 100$  nm), but the number of scattering events per volume will be largest inside the atomic wire itself due to the large current density. As a consequence, the average lattice vibration energy at the narrowest cross-section will be larger than anywhere else in the contact, which can be viewed as an increased local effective temperature,  $T_{\text{eff}}$ . This elevated local temperature can lead to the rupture of the contact, and is therefore an important parameter.

There have been several experimental attempts at measuring this local effective temperature inside metallic point contacts, but it has been difficult to obtain quantitative results. van den Brom *et al* [7] have exploited the switching rate between two different configurations in atomic sized contacts. When the energy barrier between the two configurations is low enough (which is often found on the verge of an atomic reconstruction) the local temperature can activate the jumps between the two levels, and the switching rate is determined by the ratio of the effective barrier and the thermal energy. To obtain the effective temperature from this switching rate an estimate of this barrier is required, which is difficult in view of the unknown atomic configurations. In order to circumvent this problem the switching rate between the two states was followed while changing the bias voltage and the bath temperature independently [8]. A comparison between the changes in the switching rates in these two cases would provide a calibration of the relation between the bias voltage and the effective temperature. However, the thermal expansion in the electrodes due to the changing temperature changes the atomic configuration considerably, making it difficult to draw definite conclusions.

Here we discuss measurements of the fracture rate of atomic chains as a function of the voltage bias. The advantage over previous work on  $T_{\text{eff}}$  in atomic-sized conductors is that they are free of lattice imperfections and impurities and the structure is known, except for the configuration at the end points. The energy barrier that has to be considered in the process is therefore less complex. Moreover, it is possible to consider chains of various lengths, which provides us with a control parameter of the point contact geometry.

The paper is organized as follows. After some details on the experimental techniques, we show in section 3 that the breaking of an ensemble of chains cannot be described by a simple activated process. We argue (section 4) that there are a number of parameters involved that lead to a distribution of Boltzmann factors, and we show that the observed distribution in breaking voltages can be fairly well described without adjustable parameters. One of the assumptions, here, is that there is a variation in effective barriers to breaking as a result of a distribution of tensile forces in the chains. We verify this assumption in section 5 by comparison to the measured phonon mode energy in the chains, which reflects the actual tensile force in the monatomic wire. All experiments to this point were done on gold chains, and this is compared to results for platinum in section 6, which can only be qualitative for the lack of data available in the literature. We conclude (section 7) that we have a fairly good description of Joule heating in these atomic-sized conductors, and we obtain a realistic estimate for the lattice temperature at finite bias.

## 2. Experimental techniques

The experiments have been performed using the mechanically controllable break junction (MCBJ) technique [3]. In this technique one breaks a wire of the desired metal in a controlled fashion with the use of a piezo-electric element. The wire is only broken once the sample is under vacuum and the temperature in the vacuum chamber is stable at 4.2 K. Thermal contact to the sample is provided by a copper finger in order to

avoid using thermal contact gas. The advantages of the MCBJ technique are, first, a large mechanical stability due to the small mechanical loop connecting the two wire ends. This can be of crucial importance when one tries to determine the stability of monatomic chains. Second, the cryogenic vacuum without use of thermal exchange gases ascertains the absence of gas molecules in the environment that could lead to additional cooling of the contact and contamination of the metal nanowire. Our relying on cryogenic vacuum has the disadvantage that we cannot increase the temperature of the experiment much, since this would lead to a deterioration of the vacuum. The gold and platinum wires used here have a purity of at least 99.998%.

Chains of atoms were produced in the following way. During the breaking of the wire by use of the piezo-element the wire conductance decreases in steps [9], which have been shown to be due to atomic reconfigurations [10]. The last plateau in the conductance, observed just before the conductance suddenly drops to a negligible value and the wire is broken, is generally due to a contact with the cross section of a single atom [11]. When the length of this plateau exceeds the typical length for a single atom, it can be considered as a measure for the length of an atomic chain being formed [4, 12]. In order to fabricate atomic chains of a given length  $L$  the process is repeated as long as the contact breaks before the plateau (and chain) reaches the desired length. The two electrodes are pushed together again to reestablish a big contact, and a new atomic contact is pulled out. When after several attempts the desired chain-length is reached, the piezo movement is halted, and measurements on the properties of the atomic chain are started. During this procedure the conductance of the atomic contact is measured using a constant bias voltage of the order of 10 mV.

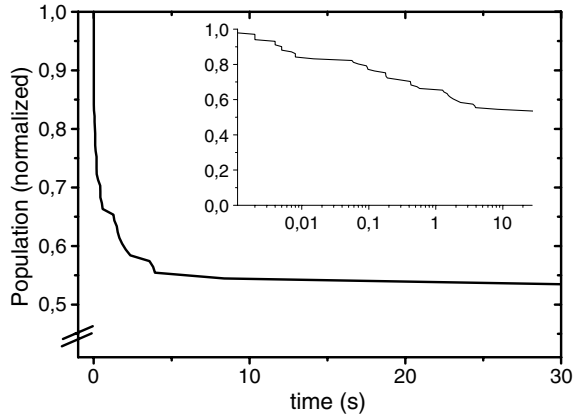
The effective length  $L$  that we will use as a parameter below refers to the length of the last plateau in the conductance, as was done in previous studies [4, 12]. The length measures the stretching of the contact from the point where the conductance first drops to the value of a single-atom contact. It is widely accepted that the starting point corresponds to a contact of one atom. Depending on the detailed evolution of the chain, a plateau length of  $L = 0.5$  nm for gold would have two or three atoms in a row, and  $L = 1$  nm would have four or five atoms. Some recent model calculations [13, 14] suggest that the structure of the contact at the starting point of a plateau can be viewed as two electrodes ending in a single atom and touching vertex-atom to vertex-atom which would make the chains one atom longer, but this remains to be verified experimentally.

## 3. The rate of decay of atomic chains

One would expect the stability of the monatomic chain to be determined by the ratio of the energy barrier against breaking,  $W$ , and the effective temperature,  $T_{\text{eff}}$ . A population,  $\mathcal{P}$ , of chains would then show an exponential decay as a function of time,  $t$ ,

$$\mathcal{P}(t) = \mathcal{P}(0) \exp(-t/\tau), \quad \tau = \frac{1}{f} \exp(W/k_B T_{\text{eff}}), \quad (1)$$

where  $f$  is the frequency by which the system attempts to overcome the barrier. In estimates and simulations given below



**Figure 1.** The number of monatomic chains remaining intact as a function of time out of an initial population of 100. The inset shows the same data on a logarithmic time-axis. The results were obtained for monatomic gold chains with an effective length of 0.4 nm, at a temperature of 4.2 K and at a constantly applied bias voltage of 200 mV.

we will take  $f = 3.5 \times 10^{12}$  Hz, a typical phonon frequency for monatomic gold chains [6, 15].

In order to investigate this stability by a simple experiment, the decay of a population of monatomic gold chains was followed as a function of time. The moment a chain of the desired length is created is taken as  $t = 0$ , and the time until the chain spontaneously breaks was stored for a set of consecutively formed chains. The evolution of the number of surviving chains as a function of time, out of an initial population of 100, is presented in figure 1. Clearly, the observed dependence is not described by the expected exponential decay. The inset in figure 1 shows that it actually more closely follows a logarithm. A logarithm can be obtained if we consider for the chains in the population a distribution of barriers, a distribution of effective temperatures, or both. Note that the characteristic time for breaking is influenced by the applied bias voltage, which is 200 mV in the example of figure 1. Near zero bias the lifetime of atomic chains at 4.2 K is mainly limited by the patience of the experimentalist.

#### 4. A distribution of Boltzmann factors

The distribution of lifetimes for given effective length  $L$  observed in figure 1 may result from a variation in the energy barrier  $W$  of the chain, which is likely to be due to variation in the tensile force. From the fact that a chain will always break when the tensile force exerted is large enough, one can conclude that the effective barrier height must decrease with force. As shown by the force measurements on monatomic chains performed by Rubio *et al* [10], the force varies strongly while pulling to form a chain, and it will sensitively depend on the atomic configurations at the connection points to the banks. Assuming a dominant lowest order (linear) term, the barrier energy can be written as

$$W = W_0 - \alpha|V| - \beta|F|, \quad (2)$$

where  $W_0$  is the equilibrium barrier energy. We have also included a linear decrease of the barrier due to electromigration

upon application of a bias voltage  $V$ . This term is motivated by model calculations by Todorov *et al* [16, 17]. Using a single-orbital tight-binding model they have shown that the barrier against breaking reduces linearly with voltages up to 1 V. More recent calculations based on density functional theory by Brandbyge *et al* [18] have shown that the electromigration force can be highly non-linear. However, for many configurations it will be a reasonable approximation.

Apart from a variation in the energy barrier we should also consider the local effective temperature at the point contact. For vanishing bias voltages the effective temperature approaches the bath temperature,  $T_0$ . Beyond a certain threshold voltage it should rise due to a voltage-driven term,  $T_V$ . Following [16] we describe the local effective temperature of the atomic contact as

$$T_{\text{eff}} = (T_0^4 + T_V^4)^{1/4}. \quad (3)$$

An estimate for the dependence of  $T_V$  on voltage can be obtained from an earlier paper by Todorov [19]. Three terms are included in the estimate:

- (1) heating by the electrons due to creation of phonons in the atomic wire,
- (2) the cooling by the electrons due to absorption of phonons, and
- (3) cooling by the thermal transport of energy away from the point contact into the metal banks.

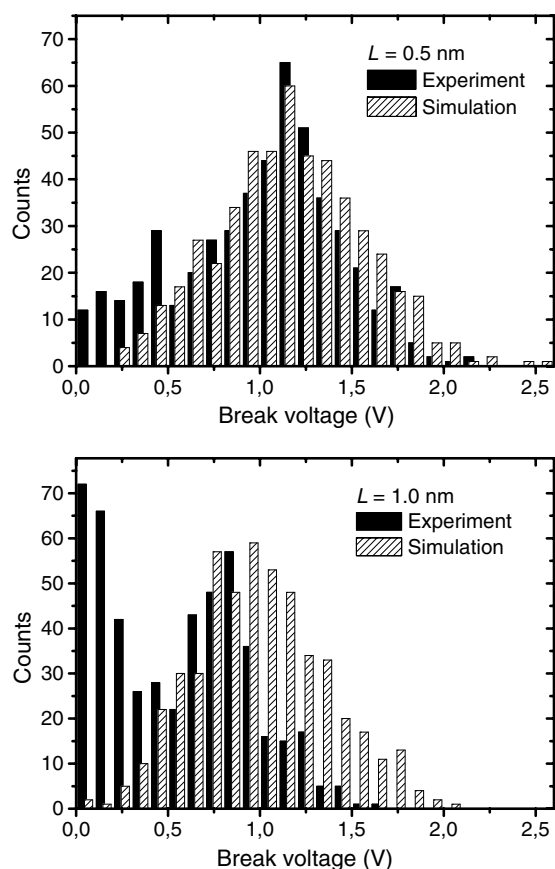
If only the first two terms are included, the temperature is simply proportional to the voltage,  $k_B T_{\text{eff}} \simeq eV$ , where it has been assumed that electrons exchange at most a single quantum of vibration energy. Note that recent experimental work by Zhitenev *et al* [20] on molecular junctions indicates that several vibrational quanta can be deposited per electron. However, this effect can be attributed to the relatively long residing times of the electrons inside the molecular bridge [21]. Earlier experimental work on phonon spectroscopy in monatomic gold chains [6] shows that multiple phonon scattering is negligibly small for these ballistic wires, in agreement with the assumption by Todorov.

An effective temperature  $k_B T_{\text{eff}} \simeq eV$  would correspond to thousands of kelvins at commonly employed bias voltages. However, the third term, the thermal conduction to the banks, limits the heating considerably. It is more difficult to make precise estimates, but when the behaviour of the banks is taken to follow the bulk heat conduction and heat capacity we obtain [19]

$$T_V = \gamma \sqrt{L|V|}, \quad (4)$$

where  $\gamma$  is a proportionality constant given as  $\gamma = 60 \text{ K V}^{-1/2} \text{ nm}^{-1/2}$  and  $L$  is the length of the chain. This was qualitatively confirmed by an independent approach by Chen *et al* [22].

In order to investigate experimentally the effect of bias voltage heating on the stability of the chains, taking a distribution of wire properties into account, we proceeded as follows. First chains of the desired length are produced following the procedure described above. This is done at a bias voltage of 10 mV, a value which is below the typical electron-phonon excitation energy [6]. This ensures that the effective temperature in the point contact will remain close to the bath



**Figure 2.** A distribution of the number of gold atomic chains as a function of bias voltage at which they were observed to break. The upper panel shows the experimental and simulated result for 500 chains with  $L = 0.5$  nm long at a temperature of 4.2 K, while the lower panel shows similar data for chains of  $L = 1.0$  nm long.

temperature. Once a chain has been formed we wait for 1 s to see whether the chain is indeed stable. Next, the voltage is ramped with a constant speed of about  $1 \text{ V s}^{-1}$  until the chain breaks. The bias voltage at breaking is stored and it is reset to 10 mV. The electrodes are then pushed together again to repeat the experiment for the next chain. The results for such an experiment are represented in figure 2. The top panel shows a histogram constructed from the measured bias voltages at breaking for a set of 500 gold atomic chains with  $L = 0.5$  nm. The distribution clearly peaks at 1.2 V with a full width at half maximum of 0.6 V. The lower panel shows a similar set of experimental results for chains of  $L = 1.0$  nm in length. In this case we observe two peaks in the distribution, one at low bias representing a large fraction of chains that break early, and a second at 0.8 V. A possible dependence on the voltage ramp speeds was not investigated, but earlier work found negligible influence of this parameter in atomic contacts [23].

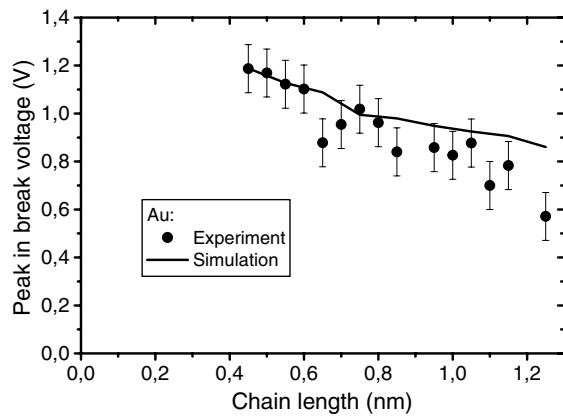
We have suggested above that the breaking of the atomic chains can be described as a thermally activated process. However, for this we need to verify that the energy barrier is not significantly modified by thermal expansion due to the rising of the local effective temperature at high bias voltage. In a test we measured two sets of 500 atomic chains. With the first set the bias voltage was suddenly increased from 15 to 800 mV once the chains had been formed. A large number of

chains was seen to break following a similar logarithmic time dependence as displayed in figure 1. With the second set we suddenly dropped the voltage from 300 to 50 mV, after which we observed not a single chain breaking. Note that a higher bias should lead to thermal expansion of the electrodes [24] and thus to a smaller tensile stress than at low bias. These two tests show that the influence of the thermal expansion on the energy barrier, if present, is dominated by the thermally activated breaking.

In order to compare the results of figure 2 with the proposed model for the variation of the energy barrier and effective temperature on bias voltage, we need realistic estimates for the constants in equation (2). We adopt the values  $W_0 = 0.738 \text{ eV}$  and  $\alpha = 0.14 \text{ eV V}^{-1}$  obtained in [16] from a non-equilibrium tight-binding calculation for a gold atomic chain. The value for  $\beta$  in equation (2) can be estimated from the results by Rubio *et al* [10]. They found that gold atomic chains typically break at a tensile force of 1.5 nN. At the point of breaking, the lifetime,  $\tau$ , of a chain has been reduced to the experimental timescale, which is  $\sim 0.1$  s in the experiments of [10]. The local effective temperature at the point contact will be given by the bath temperature in view of the low bias voltage of 10 mV used in these experiments. For  $\tau = 0.1$  s and  $T_{\text{eff}} = T_0 = 4.2 \text{ K}$  we obtain from equation (1) an average barrier of 0.011 eV at breaking. The barrier of 0.738 eV therefore nearly vanishes under the influence of a tensile force of 1.5 nN, resulting in a value of  $\beta = 0.49 \text{ eV nN}^{-1}$ .

We will now see whether the combination of these values gives a reasonable description of the experimental results of figure 2. We assume here that the only missing, i.e. not measured, parameter is the tensile force. The average tensile force on an atomic chain can be estimated from figure 1 in [10] to be  $0.95 \pm 0.15 \text{ nN}$ . We performed a numerical simulation of these data based on equations (1)–(4) and using a normal distribution of forces with a mean value of 0.95 nN and a standard deviation of 0.15 nN, which produces the distribution presented in figure 2. The peak position and width agree very well with those observed in the experiment. Note that all parameters have been obtained from independent model calculations and experimental data, so that there are no adjustable parameters. For an effective length  $L = 1 \text{ nm}$  (lower panel) the peak in the numerical simulation is slightly higher than observed. A more significant disagreement is in the width of the distribution, which is about twice as large in the numerical result, and also the peak at zero bias remains unexplained. Nevertheless, the qualitative agreement obtained using literature values for the parameters suggests that we have at least captured some of the physics involved. Thus, this analysis suggests that the broad distribution in breaking voltages is mainly caused by the large distribution of tensile forces in an ensemble of atomic chains. The processes leading to the relatively unstable chains breaking at very low voltages is as yet unclear. A possible explanation would be a large portion of chains quickly breaking when the bias voltage reaches the threshold value of the lowest phonon mode in the point contact.

In order to follow the length dependence in more detail we have constructed histograms similar to the ones shown in figure 2 for many chain-lengths. From the histograms we extract the position of the maximum of the distribution at finite bias, and plot this as a function of length. This dependence



**Figure 3.** The position of the maximum in the distribution of breaking voltages (figure 2) for monatomic gold chains as a function of their effective length. The bullets represent the experimental results obtained by fitting a Gaussian curve to each population formed by 500 chains. The curve is a numerical simulation, as described in the text.

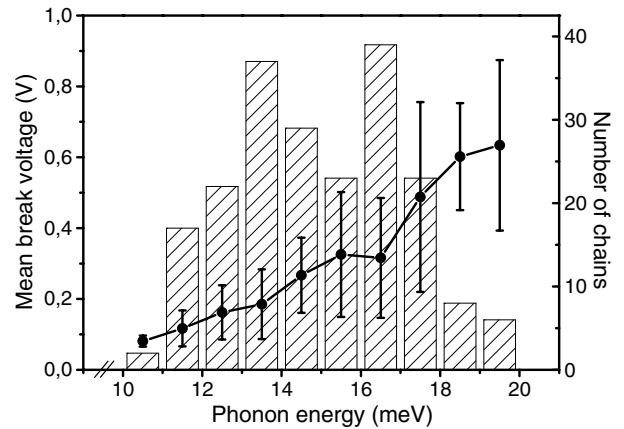
is depicted in figure 3, and shows that the average breaking voltage decreases from 1.2 V at  $L = 0.45$  nm to just below 0.6 V at  $L = 1.25$  nm.

With the same values for the model parameters as used above we obtained the curve shown in figure 3. In view of the fact that there are no free parameters, the agreement between the model and experiment is surprisingly good, although the values at greater length demonstrate a larger deviation. The reason for the deviation may be in the model or the choice of parameters. However, one aspect that we have ignored and that should become important for longer chains is the contribution of the entropy. The larger number of bonds present in longer chains will reduce the effective barrier [25].

## 5. Test of the variation in tensile forces

In order to test whether the width in the experimental distribution at higher bias voltages is the result of a variation in the tensile forces one would like to be able to measure the forces in the point contact. The MCBJ in its original configuration is not suitable to determine these, but it is possible to obtain some information in an indirect way using point contact spectroscopy (PCS) [26]. By this technique one probes the differential conductance  $dI/dV$  as a function of voltage using a small modulation superimposed on the dc bias ramp. As soon as the excess energy,  $eV$ , of the electrons shooting through the point contact becomes larger than the energy of a phonon mode inside the contact, a new channel for back-scattering sets in, resulting in a sudden reduction of the conductance. This technique was applied to atomic contacts by Untiedt *et al* [27] and to monatomic gold chains by Agrait *et al* [6], who showed that the observed phonon energy decreases when the tensile force on the chain is increased. This is as intuitively expected: as the tensile force  $F$  increases, the distance between the atoms  $a$  in the chain increases, leading to a weaker bond and a lower stiffness  $\kappa = dF/da$ . Since the observed longitudinal phonon mode energy is proportional to  $\sqrt{\kappa}$ , the phonon frequency changes accordingly.

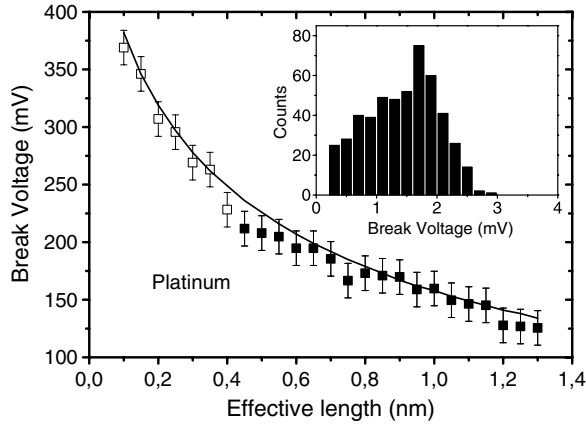
We make use of this effect in the following experiment. First we produce a chain of the desired length via the procedure



**Figure 4.** The average breaking voltage of gold chains with an effective length of 0.9 nm as a function of the observed phonon frequency (bullets). The bars indicate the number of data points used to obtain the average (right-hand axis). The standard deviation in the break voltage for each phonon frequency is represented by the size of the error bar.

described above. Next, a point contact spectrum is recorded by measuring the differential conductance as a function of bias voltage in the interval between  $-50$  and  $+50$  mV, using a lock-in amplifier. Some chains are lost during this procedure due to an increase of the effective temperature caused by the increased bias voltage. When this happens the data are discarded and a new chain is formed. After having measured the differential conductance, the bias voltage is ramped up similarly to the previous experiment, at a rate of  $1 \text{ V s}^{-1}$ . The data are stored and analysed after collecting a large set of curves. For all point contact spectra that show a clear phonon signal, the phonon frequency can be compared to the breaking voltage. The data are then sorted according to the observed phonon frequencies, and collected in bins of 1 meV wide. For the data within each bin the average breaking voltage and its standard deviation are evaluated.

Figure 4 shows the average breaking voltage as a function of the observed phonon frequencies, where the error bars on each data point represent the standard deviation. For a small fraction of about 2% of the spectra, more than one phonon frequency could be identified, and these were not taken into account in figure 4. The break voltage in the graph clearly rises as a function of phonon energy, just as is expected. For a higher phonon frequency the force constant  $\kappa$  is higher, and the chain is expected to be less strained, and thus the energy barrier to breaking is higher. The distribution of breaking voltages at each phonon energy is still quite broad. From this observation one can conclude that the tensile force indeed plays the expected role on the stability, but that there are still other parameters that influence the survival rate of atomic chains at high bias voltage. Such parameters could be variations in the shape of the leads giving rise to differences in thermal conduction and effective temperatures. Also, various atomic configurations of the leads at the connection points to the chain may give rise to different equilibrium values for the barrier at zero voltage and zero strain,  $W_0$ . This may also lead to a variation in the dependence of the barrier on bias voltage via electromigration forces.



**Figure 5.** The main panel shows the evolution of the maximum in the distribution of breaking voltages (illustrated for 500 chains of length  $L = 1.0$  nm in the inset) for Pt atomic chains as a function of length. Filled squares show the data points that are in the same interval as measured for Au in figure 3; open squares represent data points outside this interval. The full curve shows the result of the model calculation described in the text.

## 6. Platinum

Gold is not unique in forming atomic chains, and it is now known that this property is shared with Pt and Ir [28]. In contrast to Au, Pt is a metal with both a significant density of s and of d electrons at the Fermi energy. The behaviour for Pt could therefore deviate from the results predicted by the model presented above, since the theory was largely based on the single-orbital tight-binding studies by Todorov *et al* [16].

The inset of figure 5 shows a histogram of breaking voltages for 500 Pt atomic chains, measured by the same method as figure 2 for Au. Since the conductance for Pt single-atom contacts or monatomic chains is not as sharply defined near a quantum unit of conductance as is the case for Au, the length of the atomic chain is less obviously defined. This problem was discussed and successfully addressed in [28], and we employ the same approach for determining the effective chain length. Although the results in figure 5 are largely similar to those obtained for Au, they differ in some respects. First, for an effective length of  $L = 1.0$  nm the position of the maximum is now located at 0.17 V, much lower than found for Au, while the width of 0.12 V is only slightly smaller. Also, the fraction of chains breaking at very low currents is significantly smaller.

Just as for Au, one can follow the position of the maximum in the breaking currents as a function of length. Such a graph is presented in figure 5, where the filled data points represent data in the same length interval that was also measured for Au, while the open symbols are at smaller lengths. This is to emphasize that the differences in behaviour are less dramatic than a comparison of the two figures may suggest. The rapid rise towards smaller lengths may not be unique for Pt. We would like to use again equations (2)–(4) to describe the experimental results for the breaking voltage as a function of length. However, in contrast to Au most parameters in the model cannot be found in the literature. Therefore, we take a slightly different approach, and start from the assumption that all chains break as soon as their mean lifetime becomes of the order of the characteristic experimental timescale. We

further assume that the effective temperature at breaking is much larger than the bath temperature, so that  $T_{\text{eff}} \simeq T_V$ . Combining equations (2)–(4) we obtain

$$\tau = \frac{1}{f} \exp\left(\frac{W_F - \alpha|V|}{k_B \gamma \sqrt{L|V|}}\right), \quad (5)$$

where  $W_F = W_0 - \beta\langle|F|\rangle$  represents the barrier against breaking averaged over a distribution of forces. We set  $\tau$  equal to an experimental timescale of 10 ms, but the choice affects the results only logarithmically. Taking  $W_F = 0.23$  eV, (note that this is  $W_0$  reduced by the averaged strain)  $\gamma = 200$  K  $\text{V}^{-1/2}$   $\text{nm}^{-1/2}$  and  $\alpha = 0.39$  eV  $\text{V}^{-1}$ , a set of values which is within reasonable limits, the resulting curve shown in figure 5 describes the experimental data quite well. This set of values is not unique, as can be seen from inspection of equation (5): the values of  $\alpha$ ,  $\gamma$  and  $W_F$  can be scaled by an arbitrary constant. Yet we can find reasonable values for the constants and obtain a good qualitative description of the data using the same model as for Au above. For  $L \rightarrow 0$  the break voltage assumes a value  $W_F/\alpha$ , while for large  $L$  the break voltage decreases as  $1/L$ , but is expected to saturate when  $eV$  approaches the characteristic phonon energies of the chain.

## 7. Conclusions

We have studied monatomic chains for Au and Pt and find a systematic dependence of the characteristic chain-breaking voltage versus the chain length. Atomic chains sustain surprisingly large current densities, but the maximum current (or voltage) decreases as the chain length grows. We have adopted a model proposed by Todorov and co-workers and find a satisfactory agreement with the observations. Especially for gold the agreement is surprisingly good in view of the fact that we have not used any adjustable parameter. Yet there are deviations that are not captured by the model and that require further study. For Pt the general behaviour of the average breaking voltage as a function of length can also be closely described by the model, although the parameters have not been independently verified. The agreement obtained inspires confidence in equations (3) and (4), and we can now estimate the effective (lattice) temperature inside the atomic wire. It rises in proportion to the square root of the bias voltage for sufficiently large bias, and for a monatomic gold chain of length  $L = 1$  nm at  $V = 1$  V it reaches a temperature of 60 K, which is well above the bath temperature of 4.2 K.

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