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Electrical transport through atomic carbon chains: The role of contacts

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ABSTRACT

Chains of carbon atoms in the sp^1 hybridization are the one-dimensional analog of graphene. The first experimental studies of electrical transport in atomic carbon chains have shown a much lower conductivity than the quantum conductance limit. Here we explain, experimentally and by ab-initio transport modeling, the limited conductivity by studying the influence of carbon contacts in different hybridization states on the electrical properties of carbon chains. *In-situ* measurements in an electron microscope allow the synthesis and electrical characterization of carbon chains. Current-voltage curves of carbon chains, spanning between carbon contacts with sp^2-or sp^3-hybridized contact atoms, are measured and calculated. Contact atoms in the sp^2-hybridization allow up to two orders of magnitude higher current than through sp^3 contacts. Another important factor is the electron distribution in the chain which is determined by an even or odd number of atoms. On the other hand, it is shown that the overall length of the chain and strain have only minor influence on the conductivity. A current carrying capacity of up to 6.5 μA at an applied voltage of 1.5 V is measured.

1. Introduction

Chains of sp^1-hybridized carbon atoms are perfectly one-dimensional electron conductors. They have no extension in the two dimensions normal to the orientation of the chain and can therefore be considered as the 1D analog to graphene. Carbyne, the bulk modification of sp^1 carbon [1,2], consisting of an arrangement of chains, has been reported in many studies [3,4] but its stability is still subject of a debate [5]. However, isolated chains of carbon atoms [6–8] have been undoubtedly identified in several electron microscopy studies [9–14]. To our present knowledge, carbon chains are the only self-supporting one-dimensional atomic conductors with a length of more than a few atoms (besides, e.g., chains of 3–4 metal atoms [15]). This makes them interesting in the ultimate miniaturization of conducting wires.

The electrical conductivity of individual carbon chains has recently been measured [16]. It has been found that strain induces a metal-semiconductor transition, i.e., a transformation from cumulene to polyyne [17,18]. However, the electrical characteristics are still far from being understood. The measured conductivities of the chains are orders of magnitude smaller than twice the quantum conductance $2G_0 = 4e^2/h$ as would be expected for two degenerate conduction channels with unit transmission. What hasn't been studied in previous work and is described in the following is the influence of several parameters on the electrical properties of carbon chains. Besides the strain state (determining the metallic vs. semiconducting behaviour [17,18]), the length of the chain, (i.e., the number of atoms) and the question whether the chains have an even or odd number of atoms [19] are of importance. However, the particular problem is that the intrinsic transport in atom chains cannot be measured because reflections at the unavoidable contacts limit the transmission. It is therefore of paramount interest to study the current-voltage characteristics of carbon chains in different bonding configurations experimentally and to find out how the current is limited by the strain state of the chain, the number of atoms, and by the nature of the contacts. Current-voltage curves in a large bias range are recorded here for chains in different bonding configurations between carbon contacts and compared to electrical characteristics calculated by *ab initio* transport modeling. Furthermore, the current carrying capacity of carbon chains, that would be an important limiting factor in possible applications, is measured for the first time.

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2. Experimental procedure

The experiments were carried out in an *in-situ* electrical probing stage of a transmission electron microscope (TEM). The probing system (*Nanofactory*) allows electrical measurements by contacting the specimen with a piezo-driven tip while the arrangement can be observed at high resolution in the TEM [20]. As in previous studies [16,21], chains of carbon atoms were unraveled from graphenic layers by first establishing the contact between the tip and graphene, passing a high current (100 μA) for "welding" the contact, then limiting the current to approximately 10 μA, and slowly retracting the tip [16,18]. Under favourable conditions, i.e., when a robust contact is established between the tip and a graphenic structure, a carbon chain spans between the tip (often covered with graphitic material) and the graphene layer while the tip is retracted. In comparison to the electrical characterization of larger objects (such as nanotubes) with the Nanofactory stage, the contact point is of atomic size and not hidden by the bulky object. For establishing a sufficiently strong contact between the tip and graphene, a metal with high reactivity is needed [21]. The experiments were carried out with a tungsten tip and a graphene electrode. The lifetime of the carbon chains was limited by stress due to instabilities of the electrodes and by unavoidable electron irradiation. It has to be emphasized that electron irradiation limits the lifetime of the chains but not their electrical properties (the higher the electron energy and the beam intensity the shorter the lifetime of the chain until rupture). In the present setup, several successive current-voltage curves of the same chain could be recorded during their lifetime of up to 20 s at an acceleration voltage of 200 kV (experiments at 100 kV didn't show a much higher lifetime but less image resolution, most likely due to charging effects and the vibration of the chain). All carbon chains in this study span between two graphitic contacts; both ends of the chains are therefore carbon-carbon contacts.

3. Measurements of current-voltage characteristics

The first important characteristic of carbon chains that is studied here is the electrical behaviour in a large range of applied voltages. This is of particular interest since the current through the chains at low bias as shown in previous experiments [18] has often been smaller than 10 nA. This would be a serious limitation in possible applications of carbon chains as conducting wires. However, theoretical work on the quantum conductance of carbon chains has predicted a rising current above a certain threshold bias, due to resonant tunneling and the transmission through channels in narrow energy windows [18]. Fig. 1 shows two successive current-voltage curves of a carbon chain in a bias range up to 700 mV. The curve shows only slight asymmetry (i.e., non-rectifying), indicating almost similar contacts on both sides of the chain. The contact on the left hand side appears to be the cap of a single-wall nanotube; on the other side it is less obvious but is most likely such a cap-like configuration too, where the chain is bonded to a sp^3-hybridized atom (fourfold coordinated) in the cap. The whole sequence is shown in video 1 in the supplementary information.

Supplementary data related to this article can be found online at http://dx.doi.org/10.1016/j.carbon.2017.06.039.

While the first curve (Fig. 1a) shows an onset of the current rise at ±200 mV, the second (Fig. 1b) has a wide plateau where the current remains very low until, at ±500 mV, the current starts rising. However, a closer look at the plateau regime (inset in Fig. 1b) shows a first small onset at ±300 mV. Each onset of current rise indicates the presence of a transmission channel at the respective energy [18]. Furthermore, it appears that the chain first has a slight curvature (Fig. 1a) and later becomes straight (Fig. 1b). This indicates an increasing stress so that the second curve corresponds to a strained chain which is supported quantitatively by a numerical calculation (see below).

An important observation is the large variation in current at the same bias during the lifetime of a chain. This is shown in Fig. 2 where different current-voltage curves were taken at certain time intervals (1–6) from the same chain. Although the different curves show a similar trend, the current at a given bias is changing considerably. It is apparent that the temporal trend goes towards a reduction in current; however, this happens mostly in an up-down-up-down behaviour (except curve 4). From the series of images corresponding to the curves (see Video 2 in the supplementary information), it appears that the length of the chain is slightly increasing. This could be due to continuous unraveling during the recording of the series of curves. Another example is shown in Section 2 of the supplementary information.

Supplementary video related to this article can be found at http://dx.doi.org/10.1016/j.carbon.2017.06.039.

Another important characteristic is the current carrying capacity of carbon chains. This was studied by taking asymmetric current-voltage curves, i.e., starting the voltage sweep at zero or moderate negative bias (to avoid failure of the chain at large

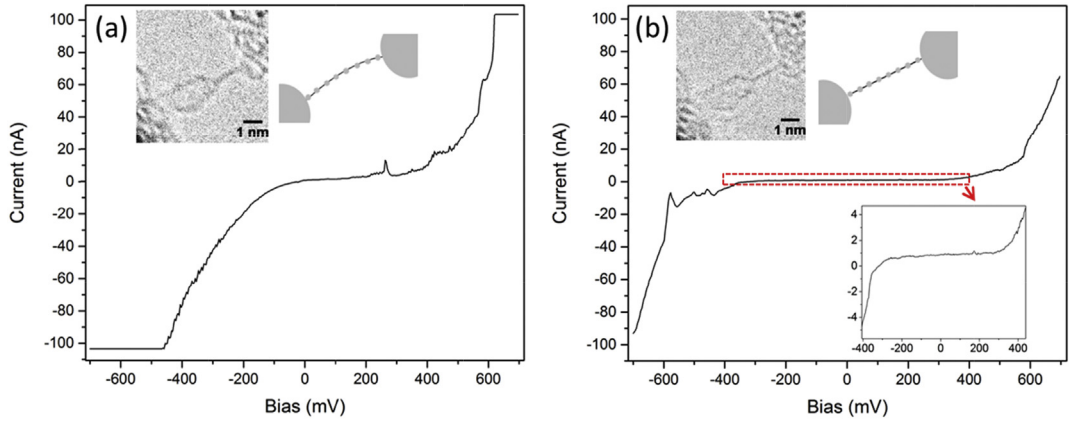

Fig. 1. Two successive current-voltage curves of the same carbon chain. The curve in (b) was recorded 2 s after curve (a). The corresponding TEM images as well as schematic drawings of the arrangements are shown in the insets. The other inset in (b) shows an enlarged region at low bias. The small peaks are due to instabilities of the contacts during the voltage sweep (within 100 m). The current was limited to 100 nA. See also supplementary video 1. (A colour version of this figure can be viewed online.)

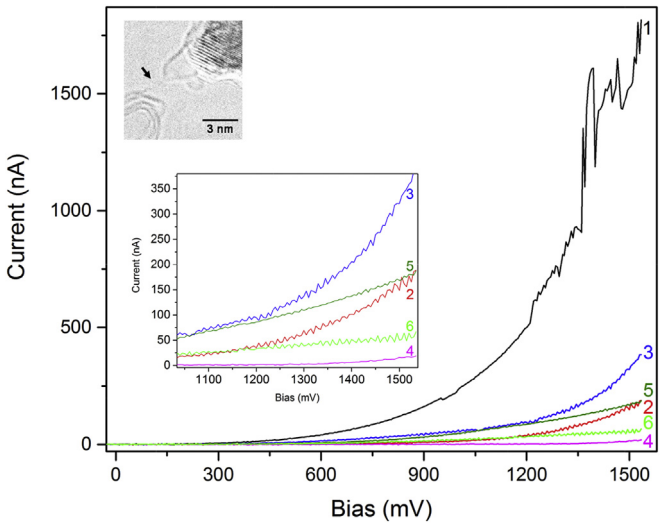

Fig. 2. Current-voltage curves from the same carbon chain at different time intervals, numbered from 1 (t = 0) to 6 (t = 10 s). The total lifetime of the chain under the electron beam was approximately 11 s. See also video 2. (A colour version of this figure can be viewed online.)

negative bias) and then increasing the bias until rupture of the chain occurred. The maximum current measured so far was approximately 6.5 μA at an applied bias of 1.7 V (see Section 3 in the supporting information). Failure of the chain always occurred at the contact and never in the middle of the chain. Fig. 3 shows an example where the current reaches 3.5 μA at a bias of 1.5 V (Fig. 3a). Another curve on the same chain (Fig. 3b) shows instabilities at high bias until the chain ruptures. Since the current in the chain is limited by the configuration of the contacts (an ideal chain would have a conductivity of $2G_0$), the dissipation of heat at the contacts could change the bonding characteristics and lead to contact resistance changes. The instabilities can also lead to a temporary interruption of the current during the rise of the bias. This can happen repeatedly until, at higher bias, the contact fails. Apparently, the contact is able to re-establish itself after rupture. The dangling end of the chain (as seen in video 1) appears to be able to close the contact again. However, the electrical characteristics may be different after a new closure.

4. Computational procedure

In order to understand the measured electronic characteristics, the quantum conductance of various carbon chains in different configurations was computed using the Landauer–Büttiker formalism and the surface Green's function matching method, after extracting the first-principles Hamiltonian and overlap matrices as implemented in the TRANSIESTA package [22] of the SIESTA code [23]. The corresponding I/V curves can thus be extracted by integration of this conductance over a specific energy window and have been calculated for various chain lengths and semi-infinite contacts (capped nanotubes and nanoribbons). Further details of the computational method are given in the Methods Section. Density functional theory (DFT) computations were performed using the SIESTA code [23,24] with a double-ζ polarized basis set of numerical atomic orbitals, GGA-PBE exchange–correlation energy functional [25] and norm-conserving pseudopotentials [26] in a real-space mesh equivalent to an energy cutoff of 300 Ry. A Fermi–Dirac distribution function with an electronic temperature of 10 meV is used to populate the energy levels. Atomic structures were allowed to relax until forces on each atom and on the unit cell were reduced to within 0.01 and 0.03 eV/Å-1, respectively. To theoretically model the current-voltage curves, the following preliminary calculations are necessary. Atomic positions and lattice parameters were geometrically optimized prior to transport calculations using TranSIESTA for the whole system with a converged number of k-point in the transport direction [27]. The system is then divided into three parts (see Section 4 of the supplementary information): a left and a right lead, and a scattering region. The Hamiltonian for each lead is calculated with a high number of k-points, again, in the transport direction. Then, TranSIESTA generates the Green's function where the interaction with the leads was introduced as self-energies for system [22]. Finally, the current is calculated for all the different bias using a tight-binding code available in the TranSIESTA package: TBTrans.

5. Computational results and discussion

The following factors have an influence on the transmission through a carbon chain:

(1) the characteristics (sp^2 vs. sp^3) at a carbon contact;
(2) the number of atoms in the chain;
(3) strain in the chain.

(1) The ends of carbon chains can be bonded either to a sp^2–hybridized atom at an open graphenic edge or to a sp^3-hybridized atom within a graphenic layer. The latter case is found quite often when a chain is attached to the closed cap of a nanotube. As expected [18], the sp^3-link leads to a lower transmission due to a

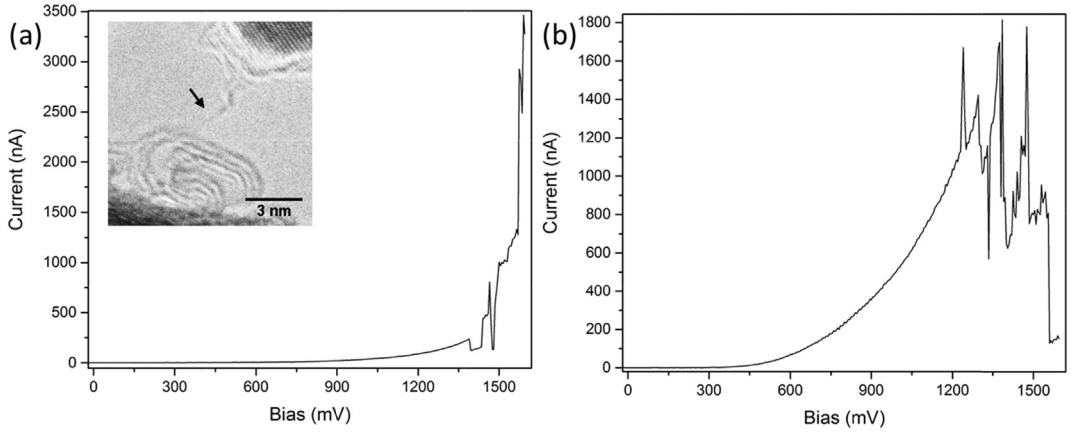

Fig. 3. Two successive I/V curves of the same chain. (a) A current up to 3.5 μA is reached at a bias of 1.5 V. (b): Rupture of the chain during an I/V recording. Considerable instabilities at the contact occur before rupture.

missing π-electron. The calculated current-voltage characteristics for three possible types of contacts (sp^2-chain-sp^2, sp^2-chain-sp^3, sp^3-chain-sp^3) are shown in Fig. 4a.

The double sp^2 configuration has two orders of magnitude higher transmission than the double sp^3 contact. Such a configuration allows currents through the chain in the microampere range at a bias of 1 V. This explains some of the measured curves where a high current of several microamperes has been observed as in Fig. 3. The transmission through a mixed sp^2/sp^3 configuration is still high but asymmetric due to the different types of contact (high transmission on one side and low transmission on the other). The chain in Fig. 2, where the chain is connected to a nanotube on one side and to a graphenic layer on the other side, could be in such a sp^2/sp^3 contact configuration. For the experimental situation shown in Fig. 1, i.e., a 10-atom chain contacted by two sp^3 links to capped nanotubes, the calculated I/V characteristics is illustrated in Fig. 4b for three different strain states. It shows a symmetry between positive and negative bias due to the presence of identical contacts in the model. The electronic transmission through the chain is the signature of a resonant tunneling transport since only a few channels at specific energy windows allow the electrons to travel between the two nanotube-based reservoirs. The curves match well both experimentally measured curves in Fig. 1. The measured curve in Fig. 1a would correspond to a chain with very low strain (which is also indicated by the very slight curvature), while Fig. 1b matches a situation with higher strain where a plateau in the curve appears at low bias.

(2) The overlap of p-orbitals along the chain determines the conductivity and is described by the model of single, double, or triple bonds. It is known that the termination with end groups determines the conjugation and, thus, the electron distribution in a carbon chain [28]. With the given boundary conditions (sp^2 vs. sp^3), an even or odd number of atoms in the chain results in different symmetries between single and triple bonds. It has already been predicted that odd-membered chains have a higher conductivity than even-membered chains [19]. Fig. 5a shows the calculated bond lengths. The π-electron density is higher on shorter (triple) bonds. Longer (single) bonds with lower electron density are thus obstacles for electron transmission. Except at the open ends, odd-membered chains have a more uniform electron density (double bonds inducing less alternation of the bond lengths in the central part of the chain) over the whole chain which facilitates charge transmission. Fig. 5b shows the calculated current-voltage curves for unstrained chains of different number of atoms. It confirms that chains with odd number of atoms have a much higher conductivity than even-membered chains.

When the number of atoms increases or decreases one by one, an oscillating conductivity should be observed. We see indirect experimental evidence for such an oscillating behaviour (Fig. 2). Since the chains are under a certain stress, the number of atoms could increase by unraveling from the graphenic contacts (since the atoms cannot be resolved in the TEM image, their number can just be roughly estimated). The increasing length changes the number of atoms between odd and even. Hence, an oscillating odd-even behaviour of the conductivity could occur. However, the experimentally measured variations are smaller than predicted for odd-even changes. This could possibly be due to a local heating at the contact when the current is high. The influence of a high vibration amplitude of the contact atoms on the conductivity has still to be investigated. As can be seen from Fig. 5b, the overall conductivity decreases slightly with increasing length, provided the even or odd number of atoms is conserved. For example, the conductivity of a 15-atom chain is less than three times lower than a 9-atom chain. The experimentally observed decreasing current is qualitatively in accordance with the expectations (longer chains should show lower conductivity). Repeated detaching and re-attaching could also lead to a changing bond characteristics but was not observed within such a series of measurements as in Fig. 2.

(3) Since the chains are mostly strained under the typical experimental conditions, purely metallic chains (that only occur when the chains are buckled) are not considered here. Nevertheless, the question arises which influence the strain state, determining the bandgap, has on the electrical conductivity. Calculated current-voltage curves for different strain states are shown in Fig. 4b (another calculation for a 13-atom chain is shown in Section 5 in the supplementary information). Even a strain of 13%, leading to a bandgap of 2–4 eV [16], reduces the conductivity by not much more than an order of magnitude. This shows that the strain cannot be responsible for the very large variations of the current that are observed in different experimental situations. Instead, the contact characteristics (sp^2 vs. sp^3) and the odd/even variation are better explanations.

The current carrying capacity of the chain is limited by the contacts. A perfectly metallic chain should have a transmission of 2 G_0 which is at least 2 orders of magnitude higher than the highest measured conductivities. In a classical picture, heat dissipates at the

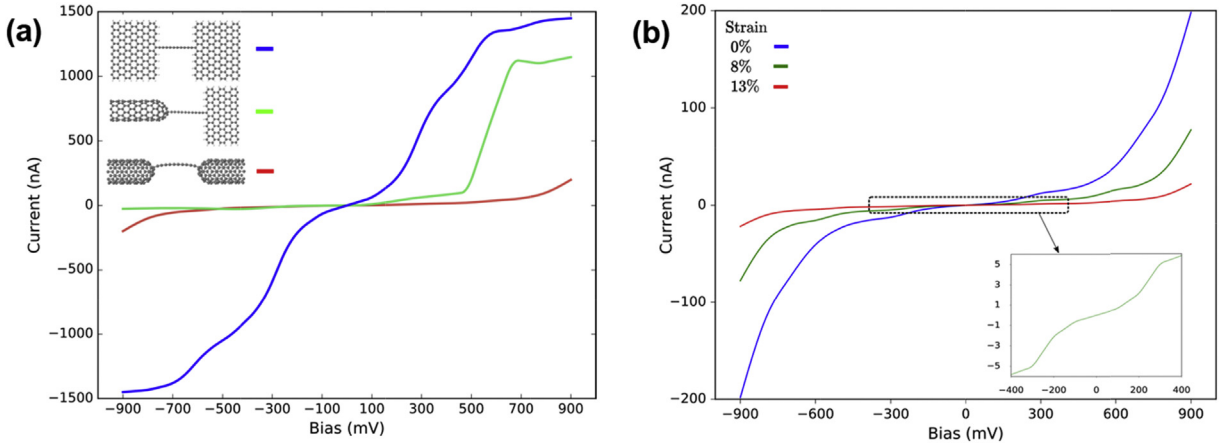

Fig. 4. (a) Calculated current-voltage curves of a 10-atom carbon chain with different contact hybridizations between the electrodes and the chain. The green curve shows the results for a carbon nanotube on one side and a graphene sheet on the other side as electrodes, making an sp^2/sp^3 configuration. The blue curve is the result of two graphene sheets as electrodes (sp^2/sp^2), and the red curve for two nanotubes (sp^3/sp^3). (b) Calculated current-voltage curve of a 10-atom chain under different strain up to 13% between two nanotube-like contacts. Both contact atoms are sp^3-hybridized. The inset shows an enlarged region at low bias for 8% strain. (A colour version of this figure can be viewed online.)

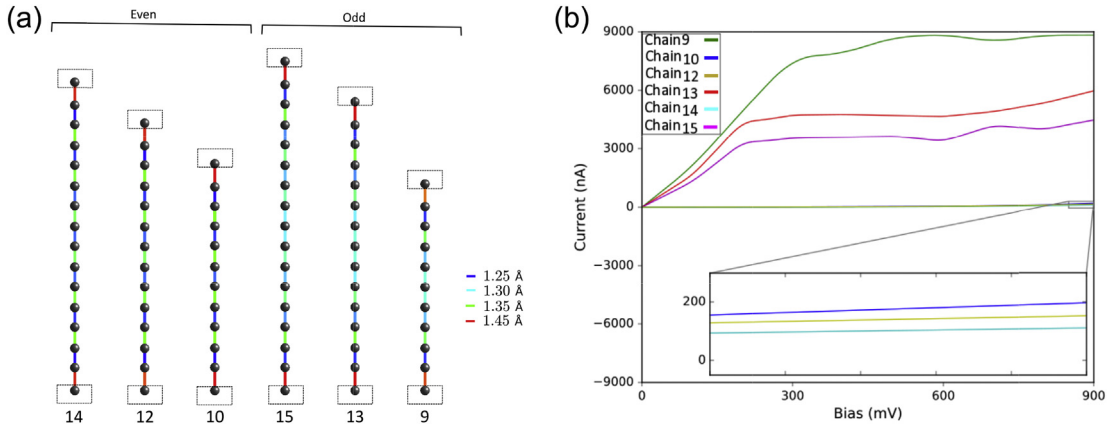

Fig. 5. (a) Calculated bond length distributions for six carbon chain lengths. The carbon atom in the grey rectangle is the contact atom of an electrode, (i.e. a CNT). The bonds are colored according to their length. (b) Theoretical current-voltage curves of different carbon chain lengths between two CNTs as electrodes: chain containing 9 carbon atoms (green), 10 (dark blue), 12 (yellow), 13 (red), 14 (light blue) and 15 (purple). (A colour version of this figure can be viewed online.)

resistivities which are the contact points where failure occurred in all observed cases. The failure of the chain at high current could thus be considered as a thermal atom displacement at the contact. Electromigration effects can most likely be neglected for carbon chains with their strong covalent bonds.

6. Conclusions

From the comparison of the experimentally measured current-voltage characteristics with the calculations, we can draw several conclusions. Major influence on the conductivity comes from the type of contacts (sp^2 vs. sp^3) and the electron distribution in the chain (even vs. odd number of atoms). The conductivity varies by up to two orders of magnitude. On the other hand, the total length of the chain and strain have only an influence of less than one order of magnitude on the conductivity. The different experimentally measured currents in different chains and the asymmetric curves thus have to be explained by different types of contacts. Odd/even variations of the numbers of atoms in the chain should have a dramatic influence on the conductivity; however, the experimental data show less variation than expected, most likely due to thermal instabilities at the contacts.

Although the majority of the experimental observations can be at least qualitatively reproduced by the calculations, several uncertainties remain. The major experimental difficulty is the impossibility to count the number of atoms in a chain and thus verifying whether the chain has an even or odd number of atoms. This is due to mechanical instabilities, e.g., the vibration of the chain in the measuring stage. Projection effects, where the chain is not exactly normal to the viewing direction, make the measurement of the length difficult. A recent study with the most advanced high-resolution electron microscopes allowed counting the carbon atoms in a chain and measuring the inter-atomic spacings [14]. However, that study was carried out under rather “silent” conditions where the chains were bridging neighbouring areas around holes in a graphene sheet Carrying out electrical measurements under these ultimate imaging conditions will certainly be a challenge since a considerably improved mechanical stability of the measuring stage would be necessary. Another experimental limitation is the displacement of carbon atoms under the energetic electron beam. This leads to a limitation of the lifetime of the chains. Imaging at lower electron energy (60 keV), below the displacement threshold, showed much longer lifetimes of the chains [14].

The results of this study show that carbon chains can only serve as efficient conductors when they are connected to sp^2-hybridized carbon atoms. The chains can carry at least 6.5 μA under suitable contact configurations (see Section. 3 in the supplementary information). Nevertheless, the limits of quantum conductivity ($2G_0$) for an uncontacted chain are two orders of magnitude higher. The even/odd number of atoms, leading to variations of the conductivity, is another restriction that could make the application of carbon chains in circuits difficult. Future experiments on carbon chains connected to metals contacts will shed more light on their suitability for applications as atomic conductors.

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Appendix A. Supplementary data

Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.carbon.2017.06.039.

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