Conductance of atom-sized Pb contacts

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Abstract. The contact formation of a metallic tip approaching Pb thin films supported on Ag(111) substrates is investigated with a cryogenic scanning tunnelling microscope. Although contacts to thicker Pb films are formed rather abruptly, the transition between tunnelling and contact is gradual for the first Pb monolayer on Ag(111). This behaviour may be understood in terms of different vertical bonding strengths due to a charge-transfer-induced surface dipole. Owing to the gradual evolution of tip–surface contacts on the first Pb(111) monolayer, imaging can be performed at contact. Furthermore, we show that for atomic-sized Pb contacts, the interpretation of peaks in conventional conductance histograms in terms of single-atom point-contact conductances yields an overestimation of contact conductances.

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1. Introduction

The electron transport properties and mechanical characteristics of atomic-sized metallic contacts are of fundamental interest in view of future nanoscale device technologies. Proximity probes like the scanning tunnelling microscope (STM), metal break junctions and related techniques, together with computational methods for simulating tip–sample interactions with atomic detail, have made it possible to address this issue [1]. Tip–surface point contacts are known to exhibit a jump of the conductance [2]–[5]. When stretched to the point of breaking, their conductance decreases in discrete steps. The shape of this staircase is material dependent and is related to the electronic and mechanical properties of the contact region [6]. The conduction in such systems is usually discussed in terms of the Landauer formula [7, 8]. Using a suitable set of quantum states, so-called eigenchannels, the low-temperature linear conductance of a point contact can then be written as \( G = G_0 \sum_i T_i \), where \( T_i \in [0, 1] \) are transmission probabilities of the eigenchannels and \( G_0 = 2e^2/h = 77.5 \mu S \) is the quantum of conductance. Here, \( h \) is the Planck constant and \( -e \) the electron charge. Much current research aims at measuring, understanding and controlling these transmission probabilities and their variation with geometric structure, electrode material, electrode magnetization, mechanical strain, etc. Taking advantage of the imaging capability of the STM, recent experiments on individual adsorbed atom (adatom) [5], [9]–[11] and on single-molecule [12]–[14] contacts showed that these contacts can reproducibly be made without structural changes of tip or sample.

Here we report a study into the conductance \( G \) of a Pb tunnel tip contacting Pb(111) thin films supported on Ag(111) substrates. The contacts are found to show a reproducible variation from tunnelling to the contact regime with purely elastic deformations of tip and sample. So far, such behaviour has not been observed on close-packed fcc metal surfaces at low \( V \), where contacts are known to quite reproducibly result in material transfer from tip to sample [5]. The transition between tunnelling and contact is found to be more gradual for the first Pb(111) monolayer (ML), while contact to thicker films is more abrupt. This behaviour may be understood in terms of different vertical bonding strengths due to a charge-transfer-induced surface dipole, which increases the stiffness of the Pb–Ag bond compared to a Pb–Pb bond. For the first Pb(111) ML, it is shown that owing to the gradual character of the tip–surface contacts, contact imaging can be performed.

2. Experiment

Measurements were performed with a home-built STM operated at 5 K in ultra-high vacuum conditions. The tunnelling voltage \( V \) was applied to the sample. Ag(111) single-crystal surfaces were prepared by repeated Ar\(^+\) sputter/anneal cycles. Pb films were obtained by room-temperature deposition from a tungsten crucible with a deposition rate of 1 ML min\(^{-1}\). Electrochemically etched W tips were prepared by annealing cycles and indenting into Pb islands, thereby covering the tip apex with Pb [15, 16]. Throughout the article we refer to these tips simply as Pb tips. The current \( I \) versus tip excursion \( z \) was measured by opening the feedback loop and driving the tip towards the surface by \( \approx 2 \) Å at velocities ranging from 0.5 to 2 Ås\(^{-1}\). The experimental setup of Limot et al [17] was used to avoid a significant voltage drop at the current preamplifier.
3. Results and discussion

Pb grows on Ag(111) in the Stranski–Krastanov mode [18, 19] with an initial 1 ML thick wetting layer (WL) that exhibits a hexagonal Moiré-type modulation with a (\(\sqrt{19} \times \sqrt{19}\)) \(R\ 23.4^\circ\) supercell [20]. The in-plane lattice constant of the Pb WL corresponds within 99% to the (111) in-plane lattice constant of bulk Pb, 3.5 Å. At higher coverage, flat-top islands of distinct heights are formed. The in-plane lattice constant on the Pb islands corresponds to that of bulk Pb. We number the film thicknesses, including the WL in MLs.

Figure 1 shows an atomically resolved image of the Moiré pattern observed on a 6 ML Pb island. The colour scale corresponds to a height range of 0.23 Å. On the Pb islands, the Moiré pattern can be observed for film thicknesses as large as \(\approx 35\) ML [21]. Altfeder et al [22] reported that the Moiré pattern in multilayers is caused by lateral adiabatic changes of the electron scattering-phase shift located at the adlayer/substrate interface rather than geometric modulation of the films.

For typical tunnelling conductances \(G\) in the range of \(\approx 10^{-5} – 10^{-2} G_0\) \((V = 100\ mV)\), the apparent height of the Moiré superstructure is \(\approx 0.1\ \text{Å}\) on the WL and somewhat smaller on Pb islands. The increased apparent height of the Moiré pattern as shown in figure 1 for a conductance of \(G = 0.09 G_0\) indicates deviations of \(G\) as a function of tip excursion \(z\) from purely exponential behaviour at conductances larger than \(10^{-2} G_0\), and will be discussed below.

For contact measurements on pristine noble metal (111) surfaces using low voltages, \(G(z)\) traces show a strictly exponential behaviour in the tunnelling regime up to the point where a sharp jump to contact (JTC), random in nature, occurs [4]. Usually, the tip–apex atom is transferred to the surface during this process. In the contact range, \(G(z)\) saturates and stays rather constant. In contrast, the conductance over single Ag (Cu) adatoms on Ag(111) (Cu(111)) shows a smooth and reproducible elastic transition from tunnelling to the contact regime [5].

For the Pb tip–surface contacts studied here, more than 200 contacts can be made with well-formed Pb tips without material being transferred between tip and sample. While contacts acquired in a sequence at the same location are highly reproducible, contacts on different positions of the Moiré pattern result in different shapes of the contact traces. The appearance of the contact traces ranges from very smooth behaviour, where no sign of a JTC is observed, to...
Figure 2. $G(\Delta z)$ traces of atomic-sized contacts on (a) 6 ML Pb and (b) the WL. To quantify the scatter of the traces, probability distributions were calculated at each value of $\Delta z$ and used to colour the data points (colour scale as inset to (b)). Negative values of $\Delta z$ correspond to reduced tip–sample distances. Set point: $I = 250 \text{nA}, V = 0.1 \text{V}$. A total of 80 conductance traces were acquired alternately on the two terraces, throughout the Moiré supercell. (c) Histogram of the conductance traces $G(\Delta z)$ from (a) (light blue area) and (b) (dark blue line).

JTC characterized contacts as also found on noble metal (111) surfaces [2, 5, 23]. In addition to the variations with lateral position, there are distinct differences of the contact traces acquired on the WL compared with contacts made on thicker Pb films.

Unless stated explicitly, all presented contact traces were not accompanied by material transfer between tip and sample, which was checked by repeated topographical imaging of the surface.

3.1. Thickness dependence of Pb contacts

Figures 2(a) and (b) show the conductance $G$ versus the tip displacement $\Delta z$ acquired on (a) 6 ML Pb and (b) the WL. A total of 80 conductance traces acquired alternately on the two film thicknesses is shown. After each individual contact trace, the tip was laterally moved onto the other film thickness where the next contact trace was acquired. The traces were taken throughout the Moiré supercell, without noticeable irreversible change of the tip configuration. It is found that the transition region shows a more pronounced step-like behaviour with a larger variety of the conductance traces on the 6 ML Pb film (figure 2(a)) as compared with the WL (figure 2(b)). Similar results were found for the comparison of contact traces on the WL and the 3 ML Pb.
Here we focus on thin Pb films with thicknesses \( \leq 6 \) ML and voltages \( V \leq 200 \) mV, so as to rule out any impact of quantum well states on the measured conductances \([24, 25]\). For the WL the transition from tunnelling to contact is very smooth and also more homogeneous throughout the Moiré supercell, as can be inferred from the reduced variation of contact traces in figure 2(b). To further illustrate the difference between the contact spectra acquired on the different film thicknesses, \( G(\Delta z) \) histograms of the contact traces are shown in figure 2(c). The dark blue line denotes the \( G(\Delta z) \) histogram of the WL. The smooth \( G(\Delta z) \) traces result in a histogram with a very flat characteristic, where no clear discrimination between the tunnelling and the contact regime is obvious. In contrast, the \( G(\Delta z) \) histogram of the 6 ML Pb film (light blue area) shows a clear step-like onset at the transition to the contact regime. The analysis of Pb conductance histograms on film thicknesses beyond 1 ML will be discussed in section 3.3.

We assign the differences of the conductance traces to the different atomic species in the second layer and suggest that the peculiar vertical bonding strength of the Pb(111) surface layer atoms is the origin of the observed differences of contact traces. Although the Pb surface atoms of the WL are vertically bonded to Ag substrate atoms, the surface layer atoms of films with ML > 1 are vertically bonded to Pb atoms. By means of electrochemical underpotential deposition experiments, it has been shown that the Pb–Ag bonding energy is 0.3 eV larger than that of a corresponding Pb–Pb bond \([18]\). This increase in binding energy has been shown to be related to the charge transfer effects between the WL and the Ag(111) substrate \([26]\). Assuming that the vertical bonding strength of such a Pb–Pb bond must be between the limiting values of the bonding strength of a single Pb\(_2\) dimer and that of a nearest-neighbour bond in bulk Pb, which corresponds to 0.84 and 0.34 eV, respectively \([27, 28]\), it may be inferred that the Pb–Ag bonding strength is larger by \( \approx 35 \) – 90%. Therefore, it is expected that the stiffness of the vertical bond of the WL to the Ag(111) surface atoms is enhanced.

A possibly related result was observed for single Ag (Cu) adatoms on Ag(111) (Cu(111)), where the origin of the observed smooth contact traces is a redistribution of surface charge due to the Smoluchowski effect that creates a surface dipole that enhances the bonding of the adatom \([5]\). Hence, the atomic positions are only slightly relaxed during the transition from the tunnelling regime to point contact, which is in sharp contrast to the situation on the flat noble metal (111) surfaces, where the tip apex was routinely fractured and a sudden JTC was observed. The reason is the larger stiffness of the adatom bond to the surface. It is found that the surface dipole roughly doubles the elastic constants as compared to the value found on flat surfaces \([29]\).

### 3.2. Imaging at contact

Taking advantage of the very smooth characteristics of the contact traces on the WL, it is possible to perform contact imaging. Figure 3 displays the evolution of constant current STM topographs spanning the range from (a) 0.16\( G_0 \) to (f) 1.26\( G_0 \). At conductances of \( \approx 0.25G_0 \) the corrugation of Pb atoms is reversed. Comparing figures 3(a) and (b) (0.43\( G_0 \)), the Pb atoms appear as protrusions in (a), whereas they appear as depressions in (b). Further increase of the current results in a triangular-shape-like appearance of the WL hollow positions and increased apparent heights. A similar effect of corrugation reversal has been observed for manipulated-atom images \([30, 31]\). These images were obtained by rastering a Co adatom over a Cu(111) surface, using the tip-induced local potential to trap the Co atom under the rastering probe tip. It was concluded that, due to adhesion forces, the Co atom did not precisely follow the tip, but

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hopped to the fcc or hcp binding sites nearest the moving tip. As there is no adatom involved in the acquisition of the contact images presented here, we assign the observed corrugation to the lateral elasticity of the apex atom of the tip, which, while rastering the surface, prefers to reside on the hollow position of the Pb lattice. Hence, when scanning on top of a Pb atom, the apex atom is laterally attracted and deflected towards the nearest hollow position. This causes the STM electronics to approach the tip towards the surface in order to maintain a constant current. Therefore, the on-top position appears as depressions. On these grounds the increased resolution with increased conductance may be understood in terms of enhanced attractive (repulsive) forces of the hollow (on-top) position with increased proximity of tip–apex atom and sample, so that the deflection of the apex atom as a function of lateral position becomes more inhomogeneous. As an additional feature, the Moiré pattern is observed in contact images too. The apparent height of the hollow positions is modulated according to the \((\sqrt{19} \times \sqrt{19}) \ R 23.4^\circ\) supercell. However, from the present data it appears difficult to distinguish whether this contrast reflects just real height differences due to the corrugation of the WL, or is an indicator of preferred binding sites as was suggested for Co on Cu(111) [30]. Note that, in contrast to Co on Cu(111), we do not observe a three-fold symmetry, which can be understood in terms of the Moiré supercell where Pb atoms are not in registry with the Ag(111) lattice.

3.3. Analysis of Pb conductance histograms

For a quantitative comparison of atomic-sized contacts made of different materials, the conductance traces are often represented by a single value, the contact conductance \(G_c\). \(G_c\) may be analysed using conductance histograms of large numbers of \(G(\Delta z)\) traces [1]. For noble metals the conductance histogram shows a clear peak at \(G_c\) owing to the flat-top step-like behaviour of \(G(\Delta z)\) in contact. However, for materials where the conductance shows a finite slope in the contact regime, the determination of \(G_c\) using conductance histograms is more difficult. Figure 4 shows the data of a representative series of 223 conductance traces.
bridging the transition between the tunnelling and the contact regime. These data were acquired consecutively on a 3 ML Pb film with the same tip. Contact traces acquired on 6 ML Pb, using the same voltage, show similar behaviour (see figure 2(a)). Contacts were made at different sites of the Moiré pattern. The area shaded light blue in figure 4(a) indicates the variability of the conductance measurements and encloses all 223 $G(\Delta z)$ contact traces. Here the conductance versus tip displacement is displayed on a logarithmic scale. Four representative contact traces are highlighted, showing the variety of elastic Pb contacts. The random character of the contact traces may be understood in the light of density functional theory (DFT) structure simulations, where it was shown that the JTC on Au(111) strongly depends on whether the tip is positioned on top of a surface atom or over a hollow [32]. In the following, the different regimes of the contact traces are discussed.

The exponential variation of the tunnelling current is usually characterized by the apparent barrier height $\phi_a$:

$$I \propto \exp(-1.025 \sqrt{\phi_a z}),$$

(1)
where $\phi_z$ is in eV and $\tilde{z}$ (the tip–sample distance) is in Å. For the Pb–Pb tunnelling junctions studied here, we find for $G < 10^{-2}G_0$ a constant $\phi_z$ in the range of 3.5–5 eV, characteristic for metal–metal tunnelling junctions. Here $\phi_z$ depends on the tip, film thickness and applied bias [33]. $\phi_z$ starts to increase $\approx 0.5–1$ Å before the contact is reached up to $\approx 7–8$ eV. Concomitantly, the variability of the $G(\Delta z)$ traces in the tunnelling regime recorded throughout the Moiré supercell increases, i.e. for increasing conductance the light blue shaded area in figure 4(a) gets wider. This marks the beginning of the transition region in $G(\Delta z)$ measurements and explains the enhanced corrugation of the Moiré pattern, as shown in figure 1.

In the transition region, $G(\Delta z)$ shows a rich structure (see e.g. the dark blue trace in figure 4(a)), which makes it difficult to characterize this range by an assignment of a single-valued slope. However, as a general result, we find that at conductances of $\approx 0.1G_0$ the slope of the conductance traces increases and the transition region is entered. The transition region is then followed by the contact regime, which shows an approximately constant slope (on the logarithmic scale) that is significantly smaller than the slope in the tunnelling regime.

In addition to using conductance histograms for evaluating $G_c$, other schemes have been used. For single-adatom contacts, Limot et al [5] defined $G_c$ by the intersection between the experimental curve and the linear extrapolation of $\ln(G(\Delta z))$ versus $\Delta z$ at large tip–sample separations. For the present Pb data, the point of intersection lies in the transition range for some of the $G(\Delta z)$ traces. Néel et al [11], Wang et al [14] and Berndt et al [34] used the conductance right after the JTC, which was defined as the point of intersection of linear fits to the transition and contact ranges of $\ln(G(\Delta z))$ versus $\Delta z$. Due to the rich structure of the transition range in this study, we modified this latter approach and performed a local fit to the transition range close to the contact regime, where the slope approaches a constant value. The resulting $G_c$ are highlighted by diamonds in figure 4(a) for some typical contacts. Figure 4(b) shows the histograms of $G_c$ (dark blue) derived from the 223 contacts, and of $G(\Delta z)$ (light blue) from the same data set. A Gaussian fit to the two distributions in the range from 1.0 to 2.1$G_0$ yields maxima at 1.35$G_0$ for the $G_c$ distribution and at 1.65$G_0$ for the $G(\Delta z)$ histogram. The shift by $0.3G_0$ may be understood in terms of mechanical strain, inducing a finite slope of the $G(\Delta z)$ traces in the contact regime and shifting the peak structure towards larger conductances [6].

More precisely, on a logarithmic scale the contact traces highlighted in figure 4(a) show a rather constant slope in the contact region, due to elastic deformations and mechanical strain in the junction [6]. In the transition region the slope is larger. Hence, if all conductance traces were to result in the same slope in the contact regime, the $G(\Delta z)$ histogram would be expected to show a step-like onset at $G_c$. Due to the scatter of $G_c$ in different measurements, this onset is smeared. A maximum of the histogram is reached where nearly all conductance traces have entered the contact range with its reduced slope. This behaviour can be seen in figure 4(b), where the peak in $G(\Delta z)$ occurs at the trailing edge of the $G_c$ distribution. Summarizing this issue, from $G(\Delta z)$ histograms $G_c$ is overestimated by $\approx 20\%$ in this study owing to a non-zero slope of $G(\Delta z)$ in the contact regime.

2 The range of the tip excursion was kept fixed during the measurements. Hence the significance of the histograms is reduced for conductances exceeding $G = 2.1G_0$, which is the lowest measured conductance at $\Delta z = -2.6$ Å (see the light blue area in figure 4(a)). However, the relevant finding of the mismatch of $G_c$ deduced from simple conductance histograms as obtained by mechanical break junction or STM experiments and the explicit assignment of $G_c$ as the endpoint of the transition from tunnelling to contact is unaffected.

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Our result $G_c = 1.35G_0$ is in good agreement with the conductance histograms of recent electrochemical fabricated atomic-sized Pb contacts, where no mechanical strain forces are present and which show a prominent peak at $G_c = 1.4G_0$ [35]. Earlier conventional break junction experiments led to conductance histograms with a peak at $G \approx 1.7G_0$ which again agrees with our result from Pb films with thicknesses exceeding 1 ML [1, 36].

3.4. Role of the tip

Finally, we comment on the influence of Pb tips on the contact measurements. Figure 5 shows the conductance traces measured on the WL with two nanoscopically different Pb tips. The dark blue data points denote $G(\Delta z)$ for 30 contacts acquired throughout the Moiré supercell on the WL of Pb/Ag(111). During the acquisition of the conductance trace highlighted in red, an irreversible tip switch occurred. Material was transferred from the tip to the surface (as evidenced by STM topographs), thereby changing the nanoscopic structure of the tip apex. After the material transfer, the shape of the conductance traces changed (light blue). The new nanoscopic structure of the tip favours a smooth transition from the tunnelling to the contact regime throughout the Moiré supercell.

It is clear that tip shape has a significant influence on the contact traces and that a certain tip geometry seems to persist until material transfer occurs. Pb tips that preferentially show a very smooth transition from the tunnelling to the contact regime on the WL appear to be more stable than other tip configurations. For tips that preferably show a JTC on the WL, the difference of the contact traces on the WL and Pb islands is not as pronounced. Although the stability and the shape of the contact formation are significantly affected by the atomic structure of the tip apex, we did not find an accompanying tip dependence of the resolution of tunnelling images or the shape of tunnelling spectra.
4. Conclusion

Pb(111) films deposited on Ag(111) substrates may be contacted with an STM tip without irreversible structural changes of the tip or the sample. Contact to the first monolayer of Pb shows a more gradual transition between tunnelling and contact, whereas contact to thicker Pb films is more abrupt. This behaviour is explained in terms of different vertical bonding strengths due to a charge-transfer-induced surface dipole. For the first Pb(111) ML, it is shown that due to the gradual character of the tip–surface contacts using Pb tips, contact imaging can be performed. For film thicknesses exceeding 1 ML, contact conductances of $1.4 G_0$ are observed. Furthermore, we have demonstrated that the peak position in conventional conductance histograms deviates from this value.

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References

[1] Agraiñ N, Yeyati A L and van Ruitenbeek J M 2003 Phys. Rep. 377 81–279
[2] Gimzewski J K and Möller R 1987 Phys. Rev. B 36 1284
[3] Dürlig U, Züger O and Pohl D W 1990 Phys. Rev. Lett. 65 349
[4] Olesen L, Brandbyge M, Sørensen M R, Jacobsen K W, Lægsgaard E, Stensgaard I and Besenbacher F 1996 Phys. Rev. Lett. 76 1485
[5] Limot L, Kröger J, Berndt R, Garcia-Lekue A and Hofer W A 2005 Phys. Rev. Lett. 94 126102
[6] Cuevas J C, Yeyati A L, Martín-Rodero A, Bollinger G R, Untiedt C and Agraïñ N 1998 Phys. Rev. Lett. 81 2990
[7] Landauer R 1957 IBM J. Res. Dev. 1 223–31
[8] Büttiker M, Imry Y, Landauer R and Pinhas S 1985 Phys. Rev. B 31 6207
[9] Yazdani A, Eigel D M and Lang N D 1996 Science 272 1921–4
[10] Néel N, Kröger J, Limot L, Palotas K, Hofer W A and Berndt R 2007 Phys. Rev. Lett. 98 016801
[11] Néel N, Kröger J and Berndt R 2009 Phys. Rev. Lett. 102 086805
[12] Néel N, Kröger J, Limot L, Frederiksen T, Brandbyge M and Berndt R 2007 Phys. Rev. Lett. 98 065502
[13] Schull G, Frederiksen T, Brandbyge M and Berndt R 2009 Phys. Rev. Lett. 103 206803
[14] Wang Y F, Kröger J, Berndt R, Vázquez H, Brandbyge M and Paulsson M 2010 Phys. Rev. Lett. 104 176802
[15] Hla S W, Braun K F, Iancu V and Deshpande A 2004 Nano Lett. 4 1997
[16] Bauer E, Poppa H and Todd G 1975 Thin Solid Films 28 19
[17] Limot L, Maroutian T, Johansson P and Berndt R 2003 Phys. Rev. Lett. 91 196801
[18] Takayanagi K, Kolb D, Kambe K and Lehmpuhl G 1980 Surf. Sci. 100 407–22
[19] Rolland A, Bernardini J and Barthes-Labrousse M 1984 Surf. Sci. 143 579–90
[20] Ast C R, Pacile D, Papagno M, Glooor T, Mila F, Fedrigo S, Wittich G, Kern K, Brune H and Grioni M 2006 Phys. Rev. B 73 245428–6
[21] Altfeder I B, Chen D M and Matveev K A 1998 Phys. Rev. Lett. 80 4895
[22] Altfeder I B, Narayanamurti V and Chen D M 2002 Phys. Rev. Lett. 88 206801
[23] Kröger J, Jensen H and Berndt 2007 New J. Phys. 9 153
[24] Jaklevic R C, Lambe J, Mikkor M and Vassell W C 1971 Phys. Rev. Lett. 26 88
[25] Becker M and Berndt R 2010 Phys. Rev. B 81 205438
[26] Kolb D, Przasnyski M and Gerischer H 1974 J. Electroanal. Chem. 54 25–38
[27] Stranz D D 1981 *J. Chem. Phys.* **74** 2116
[28] Kittel C 1995 *Introduction to Solid State Physics* 7th edn (New York: Wiley)
[29] Hofer W, Garcia-Lekue A and Brune H 2004 *Chem. Phys. Lett.* **397** 354–9
[30] Stroscio J A and Celotta R J 2004 *Science* **306** 242–7
[31] Sperl A, Kröger J and Berndt R 2010 *Phys. Rev. B* **81** 035406
[32] Hofer W A, Fisher A J, Wolkow R A and Grütter P 2001 *Phys. Rev. Lett.* **87** 236104
[33] Becker M and Berndt R 2010 *Appl. Phys. Lett.* **96** 033112
[34] Berndt R, Kröger J, Néel N and Schull G 2010 *Phys. Chem. Chem. Phys.* **12** 1022–32
[35] Xie F Q, Hüser F, Pauly F, Obermair C, Schön G and Schimmel T 2010 *Phys. Rev. B* **82** 075417
[36] Yanson A I 2001 Atomic chains and electronic shells: quantum mechanisms for the formation of nanowires
   *PhD Thesis* Universiteit Leiden, The Netherlands