9 SCIENTIFIC HIGHLIGHT OF THE MONTH

Nanowires: electronic and ionic structures, cohesive and transport properties

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Abstract

The physical properties of nanowires reflect the quantum mechanical phenomena due to the confinement of the valence electron wave functions in the plane perpendicular to the wire axis. For example, the electrical conductance will be quantised. Recently, it has been realized that the characteristic electronic structure has also a direct influence on the ionic structure of the nanowire and it is not possible to separate cohesive properties and electronic properties such as conductance and capacitance.

9.1 Introduction

There is intense current interest in the physical properties of atomically-manipulated nanostructures. In such structures, quantum effects play an important rôle. Nanowires are leads where the electronic states are quantum confined to allow conduction in one dimension only. They can be produced *e.g.* by lithographic techniques on semiconductor interfaces resulting in two-dimensional electron gas systems. In this review we consider, however, three-dimensional metallic nanowires [1]. Experimentally, they can be produced in several different ways. The simplest scheme is to put two metallic protrusions in contact and then pull them from each other over atomic distances: a nanowire is produced which upon pulling is elongated and narrowed, until it eventually breaks. This basic mechanism is employed, for example, in the scanning tunneling microscopy (STM) studies of nanowires [2]. Pulling of macroscopic wires also produces nanowires. This can be done by using the sophisticated mechanically controllable break-junction technique (MCBJ) (Ref. [3]), but even simpler arrangements are sufficient [4, 5]. An interesting possibility is to produce nanowires by filling carbon or other kind of nanotubes [6]. In the experiments the conductance is usually monitored as a function of the elongation of the nanowire.

Moreover, in the atomic force microscope (AFM) experiments by Rubio, Agraït and Vieira [7] the conductance and the force during the formation and rupture of Au contacts have been measured simultaneously. A clear correlation between the force oscillations and the conductance steps during the elongation of the nanowire was seen.

Modeling of the formation of metallic nanowires in a STM experiment was first done by molecular dynamics simulations in which the atomic structure was solved using classical many-atom-type interaction potentials [8, 9]. The simulations showed that the elongation takes place through successive stress accumulation and relief stages reflecting rearrangements in the ionic structure. The calculated ionic structures were then used to determine the electric conductance by counting the available conductive channels. The scattering of the conduction electrons may be taken into account by solving for the transfer matrix for an *afterwards* constructed effective potential [10, 11, 9]. The conductance is then given by the Landauer formula [12]

$$G = G_0 \sum_i T_i(E_F), \tag{1}$$

where $G_0 = 2e^2/h$ is the conductance quantum and $T_i(E_F)$ is transmission probability for an electron entering the nanowire constriction with the Fermi energy E_F and within the channel (subband) i.

The weakness of the above procedure is that the direct correspondence between the cohesive and conduction properties through the valence electron structure is broken. The first-principles molecular dynamics simulations based on solving the self-consistent electron structures remedy this deficiency [13, 14, 15]. Indeed, this kind of simulations [13, 16] show that the atomic geometries at the neck can be derived from those of isolated small atomic clusters, the stability of which derives from the closed-shell structures of valence electrons. The rôle of the valence electron structure is emphasized in jellium-type models [17, 18, 19, 20, 21, 22], which completely ignore the detailed ionic structure. In these calculations the confinement of the valence electrons in the direction perpendicular to the wire results in an electron level structure, the subbands of which are gradually emptied as the wire elongates and its radius decreases. As a result, cohesive properties, such as the elongation force will show oscillations as the radius of the wire reduces. Moreover, because the subbands constitute the conductance channels, the conductance shows simultaneously a steplike behaviour in correlation with the force oscillations.

The electronic transport of nanowires exhibits similar quantum regimes as seen in the context of mesoscopic devices [12]. However, several new qualitative features arise. First, the length scales are comparable to the interatomic distances and therefore the atomic information cannot be summarized by a continuum model with an effective mass. Second, an essential ingredient in the scattering theory of the quantum transport is the contact to the external world. This means that the chemical interaction between the nanowire and its immediate environment is much stronger than, for instance, in the case of a tunneling contact. These issues are addressed by two complementary descriptions. Free electron models explain the conductance in terms of geometric characteristics of the wires in comparison with the Fermi wavelength [18, 23, 24]. The second class of models rationalize the experimental observations by focusing on the chemical nature of the atomic-size contacts. They decompose the conductance into contributions due to different atomic orbitals. A good example is the work by Lang *et al.* studying a wire of two

Xe atoms between leads described by the jellium model [25]. An almost quantitative agreement with experiment was found. Another example is the study of linear carbon chains showing a conductance with an even-odd dependence on the number of carbon atoms [26].

A linear chain of atoms would be the ultimate shape of a nanowire before breaking. Their existence was predicted by Sørensen *et al.* [27] by simulations based on effective-medium-theory many-atom potentials: When pulling a Au wire along the [100] direction a linear chain of six single Au atoms appeared. Recent experiments employing electron microscope imaging [28] or the measurement of the conductance as a function of elongation [29] have also shown the formation of chains which consist of several Au atoms. A puzzling results is that both experiments predict that the interatomic distance in the chain is about 3.5 ... 4.0 Å, which is considerably larger than the bond length of 2.9 Å in bulk gold. According to the effective-medium theory or first-principles calculations the equilibrium distance is smaller than the bulk distance [27].

9.2 Electronic structure and cohesive properties

In this and in the following section we review results [22] obtained by modelling the nanowires as infinitely long cylinders of stabilized jellium. Rather similar results have been obtained with a normal jellium model for wires with r_s corresponding to the valence electron density of Na [17] and with a model which considers only the kinetic energy the electrons confined by an infinite potential barrier inside the metal wire [18, 19, 20].

In the stabilized jellium model [30], the positive ionic charge is smeared to a rigid background charge with the constant density of $n_+ = 3/(4\pi r_s^3)$ within the cylinder of radius R. In contrast to the normal jellium model, a constant correction is added to the potential inside the cylinder so that the system is stable at the bulk electron density desired. The electron structure, neutralizing the positive background charge, is solved self-consistently using the local spin density (LSD) approximation. The stabilized jellium model has been shown to give a reasonable description for the surface and void energetics of simple metals [30, 31].

The eigenfunctions $\Psi_i^\sigma(\mathbf{r})$ for the infinite cylindrical geometry have the form

$$\Psi^\sigma_{mnk_z}(r,\phi,z) = \frac{e^{ik_z z}}{\sqrt{L}} \frac{e^{im\phi}}{\sqrt{2\pi}} R^\sigma_{mn}(r), \tag{2}$$

where $m = 0, \pm 1, \pm 2, ..$ is the azimutal quantum number, $n = 1, 2, 3, ..$ is the radial quantum number related to the number of radial nodes $(n-1)$ of the radial wave function $R^\sigma_{mn}(r)$. Further, k_z is the wave vector associated to the axial z direction along which the electrons have no restriction to move, and L is the normalization length along the z axis. Thus, the electronic structure consists of one-dimensional subbands.

The subband structure is reflected in the cohesive properties of the jellium wires as a function of the cylinder radius R. For example, the surface energy σ of the Na wires shown in Fig. 1, exhibits oscillations due to the filling of new subbands. As a result, there exist cylinder radii at which the total energy per volume has a local minimum. These (meta)stable wires correspond to the magic-number jellium spheres discussed in the context of small atomic clusters [32]. Assuming that the volume of the wire is conserved one can calculate the force needed to elongate the wire

as

$$F = -\frac{dE}{dL} = -\frac{d(2\pi RL\sigma)}{dL} = -\pi R\sigma + \pi R^2 \frac{d\sigma}{dR}. \quad (3)$$

The force is shown as a function of the radius in Fig. 2. for Na wires. Negative values mean that an external force should be applied in order to elongate (and narrow) the wire, whereas at the regions of positive force the wire would spontaneously elongate and become narrower. The prominent feature is that the force shows oscillations. The amplitude of these oscillations scales approximately as $\epsilon_F(\bar{n})/\lambda_F(\bar{n})$, where $\lambda_F(\bar{n})$ is the Fermi wavelength [18]. The magnitude of force oscillations seen in the measurements for Au is well described by this estimation [7].

The AFM experiments show stress accumulation and relief stages as the nanowire elongates [7]. The conductance is correlated with the force measured so that during the stress accumulation stage the conductivity is constant and at the relief stage it decreases rather stepwise. These notions have their counterparts in the stabilized jellium model: The step in the conductance is associated with the raise of a subband above the Fermi level. Thereafter the next subband begins to empty causing the stress accumulation while the conductance will be constant (See Fig. 1 b and c). The conductance step structure with steps of 1 G_0, 2 G_0, 2 G_0, 1 G_0 seen in Fig. 1c (for the spin-compensated case) reflects the orbital degeneracies in the cylindrical symmetry. The sequence was first predicted by Bogachek *et al.* [33] and it has been seen in the measurements for Na nanowires [3].

The next step towards a more realistic description of the actual nanowires is to consider a jellium wire with variable cross section, *i.e.* a wire with a narrow neck region [18, 34]. As a matter of fact, Yannouleas *et al.* [34] have made this step within the jellium model using their computationally efficient shell-correction method. One of their main conclusions is that the cohesive and transport properties of the wires are determined to a large extent by the electronic structure at the narrowest part of the wire. This conclusion justifies the use of model with a constant (stabilized) jellium as a first approach to the problem.

9.3 Spontaneous magnetization of simple-metal nanowires

Using the stabilized jellium model we have made the surprising finding that cylindrical wires may exhibit at certain radii spontaneous magnetic solutions [21]. They appear so that the highest energy subband is totally spin-polarized when its occupancy is small enough. The spin-polarization lowers the the surface energy and causes abrupt relief stages in the elongation force (See Fig. 1 a and b). Moreover, the conductance steps of purely spin-compensated wires are divided into two steps (Fig. 1c).

The calculations predict that at very small radii the lowest subband, which in this case is the only occupied one, will be totally spin-polarized. This kind of spontaneous spin polarization has been predicted also by Gold and Calmels [35] for cylindrical wires using the exchange-correlation energy of a quasi-one-dimensional electron gas. At first sight, the result is in contradiction with the old theorem by Lieb and Mattis [36] stating that the ground-state of a strictly one-dimensional, one-subband system should be spin-compensated. However, in our case we are dealing with three-dimensional electrons interacting via the Coulomb potential, for which the Lieb-Mattis theorem is not valid.

We can analyze the appearance of magnetic ground-state solutions of simple metal nanowires by making use of the Stoner criterion of ferromagnetism in bulk metals. The occurrence of magnetic solutions in the beginning of the occupancy of each new subband would suggest the application of Hund's rules for finite systems. But the number of electron states in a subband is not limited because a jellium wire is infinite in the z direction. From the viewpoint of an infinite system it is natural to ask whether the appearance of the magnetism in the jellium wires could resemble that in bulk metallic systems, i.e., if the Stoner criterion is applicable. According to this criterion, ferromagnetism exists whenever the condition

$$I\tilde{D}(E_F) > 1, \tag{4}$$

is fulfilled. Above, $\tilde{D}(E_F)$ is the density of states (DOS) per atom in a spin-compensated system at the Fermi level and I is the Stoner parameter for the atom in question. I is an "exchange" integral which includes also the electron-electron correlation effects.

The product $I\tilde{D}(E_F)$ is plotted in Fig. 2 as a function of the wire radius R for stabilized jellium wires corresponding to Na. For the Stoner parameter I the value for a homogeneous electron gas has been used. The peaks in the figure are due to the $1/\sqrt{E}$ divergences of the DOS at the bottoms of the subbands. The filled markers mean systems for which we have found in self-consistent electronic-structure calculations stable magnetic solutions, *i.e.* the total energy of a spin-polarized solution is lower than that of a spin-compensated one. The open markers denote then stable, spin-compensated systems. The correlation between the fulfillment of the Stoner criterion and the existence of magnetic solutions is almost quantitative. It can also be seen from the figure that the region, in which the highest subband is polarized, narrows when the radius R increases indicating the recovery of the spin-compensated bulk Na.

The appearance of magnetic solutions is a consequence of the high DOS values. In the present model high DOS values reflect the confinement perpendicular to the wire and the assumed perfect translation symmetry along the wire. For more realistic finite wire geometries we expect our prediction of magnetic solutions also to be valid in the sense that the *local* DOS at the Fermi level and at the constriction will for certain radii be so high that the Stoner criterion is fulfilled. We are not aware of direct experimental observations of the magnetic structures in the case of simple-metal nanowires. The interpretation of the conductance measurements is difficult due to the scattering probabilities $T_i(E_F)$ less than unity [23] and due to the possible orbital degeneracies. However, it is encouraging that experimental evidence of this kind for magnetic "fingerprints" exists in the conductance measurements of quantum point contacts at the interface between two different bulk semiconductors [37]. Moreover, the recent conductance results for metallic carbon nanotubes may also indicate non-trivial magnetic structures [38].

9.4 Atomic chains

The rôle of the atomic structure has not been included in the jellium calculations. We have studied the ensuing effects by calculations [39] for atomic Al and Na wires with the ab initio full potential augmented plane-wave method (FLAPW) [40]. The importance of these calculations is not only in checking the stabilized jellium predictions. They also serve as simulations for metallic atomic chains which may be realized in experiments as free-standing chains as discussed in the

Introduction or as supported ones on some insulating substrates such as silicon or an ionic material [41].

We have chosen the linear Al chain as an example because the stabilized jellium model model predicts that it should have a magnetic solution when the atomic distance is close to the nearest-neighbor bulk distance of $d_{nn} = 5.41$ au. The resulting band structure is compared with the stabilized-jellium band structure in Fig. 3. The agreement is surprisingly good supporting the use of the stabilized jellium model for Al even in the present confined geometry. The polarization of the second subband accommodating the Al $3p$ electrons is the reason for the magnetic solution. The magnetic moment per atom, 0.79 μ_b, is mainly due to this subband and it should be compared with the stabilized-jellium result of 0.69 μ_b.

We have varied the bond distance in the Al chain in order to search for the total energy minimum, as well as to study the stability of the magnetization. The results are plotted in Fig. 4. The energy minimum is found at approximately $d_{nn} = 4.5$ a.u. and it corresponds to a spin-compensated solution. The magnetization appears at distances larger than 5.1 a.u. The realization of an Al chain with such relatively large interatomic distances might be experimentally possible. Namely, for example, the normal distances of metal atoms deposited on Si surfaces are of this order [41]. Moreover, the unsupported Al chain is very soft: according to our FLAPW calculations the total energy changes only by 0.05 eV when increasing the interatomic distance by 0.2 a.u. from the equilibrium bond length. Therefore it might be possible to control the spin-polarization properties of the atomic chains by varying the structural parameters of the underlying supporting surface.

The linear chain of Na atoms with a nearest neighbor bulk distance shows no spin polarization. This is also the stabilized-jellium model prediction. Only the increase of the interatomic distance to an unrealistically large one will result in a magnetic solution. In order to demonstrate the possible existence of magnetic Na wires, we have made calculations for a planar zigzag chain of Na atoms. When the interatomic distance in this kind of chain is the nearest-neighbor bulk distance and the angle formed by three adjacent atoms is about 70 degrees, a (non-degenerate) spin-polarized p-type band appears.

Our FLAPW calculations have demonstrated that atomic chains may have magnetic solutions. However, more realistic calculations taking into account the effects due to the leads in the case of otherwise unsupported chains and the effects due to the substrate for the surface-supported chains are needed to fully explore the properties of these systems.

9.5 Quantum transport

In this section we review studies [42, 11, 43, 15, 14] which apply the scattering theory of transport [12, 45] to determine the linear transport coefficients of nanowires. The conductance and capacitance are defined as the response to a time-independent and time-dependendent external bias, respectively. The scattering potential $V_s(\mathbf{r})$ is the Kohn-Sham potential obtained by a pseudopotential-plane-wave method. The transfer-matrix technique [44] is used to solve the 3D quantum scattering problem, so that the complete scattering matrix and wavefunctions are obtained [45]. The conductance G of the wire is then evaluated as a function of the scattering

energy E from the transmission part of the scattering matrix (Eq. 1). Nanowires are modeled as atomic clusters connected to two jellium leads ($r_s = 2.0$ a.u.). The clusters include diverse structures of aluminum and silicon atoms, ranging from single atoms to wires or nanoclusters.

A resonant tunneling transport regime was established for single atom contacts in Ref. [42]. The regime occurs when the contact atom is well separated from the leads so that there is a potential barrier between the atom and the both leads. The conductance is highly peaked at the scattering energy values corresponding to the atomic levels, which are now broadened, due to the atom-lead interactions, into Lorentzian resonances. When the atom-lead separation (on both sides of the contact atom) is decreased towards to the equilibrium distance the potential barriers are lowered. Thereby propagating channels are opened at the Fermi level, resulting in ballistic transport and conductance quantization.

In Ref. [11] transport properties of a linear chain of N aluminum atoms have been considered. Conductance quantizatition is seen as a function of the scattering energy E when $N \geq 2$. According to Table I the calculated resistance is systematically lower than that calculated for wires between planar electrodes [10]. The difference is due to a more abrupt contact in the latter case leading to a higher reflection of incoming electronic waves. The resistance of the atomic chains saturates for $N \geq 3$ whith the establishment of a quasi-1D behaviour. For linear chains of Si atoms a dip in the conductance at $E < E_F$ develops as N increases [43]. This reflects the energy gap between the σ and π subbands of an infinite linear Si chain.

In a microscopic conductor the discreteness of the electron density of states and the inefficient screening at distances comparable to the screening length leads to a capacitance which differs substantially from its classical counterpart. The *capacitive* response of an atomic wire is described in terms of the electrochemical capacitance $C = edQ/d\mu$ [46]. Here, dQ is the nonequilibrium charge distribution built-up in the wire due to variations $d\mu$ in the chemical potential with respect to the external reservoirs. By changing μ in the atomic junction charge is injected from the leads into the junction. The potential created by this charge induces charge polarization inside the conductor. dQ is found by solving a self-consistent Poisson equation for the characteristic potential $u(\mathbf{r}) = dV_s(\mathbf{r})/d\mu$ [46]. The screening may be approximated by a local Thomas-Fermi model.

In Ref. [14] the capacitance of different Al clusters "sandwiched" between two jellium leads has been calculated. The capacitance has been evaluated from the expression

$$C = \int_{\Omega_+} \left[\frac{dn_r(\mathbf{r})}{dE} - u(\mathbf{r}) \frac{dn(\mathbf{r})}{dE} \right] d\mathbf{r}, \tag{5}$$

where the integration volume Ω_+ is defined as the region of positive integrand values. The local density of reflected states, $dn_r(\mathbf{r})/dE$ and the total local DOS $dn(\mathbf{r})/dE$ are obtained from the scattering wavefunctions [47]. The capacitance of a five atom "tip" contact attached to one of the leads versus the distance between the leads is depicted in Fig. 5. At large distances, capacitance decreases and exhibits a geometric or classical behaviour. On the other hand, the capacitance is predicted to decrease towards to smaller distances when the separation $d < 5\mathring{A}$. This is clearly a quantum effect: the formation of the nonequilibrium charge distribution is diminished as the tunneling rate increases. The capacitance follows in this limit the reflection coefficient R of the electron waves coming from the leads, but displays more structure as seen in Fig. 6. The

diverse peaked structures correspond to excitations between the reflected channel states. The excitations may even occur at the conductance plateaus. The dependence of capacitance on the atomic structure at the contact is discussed in Ref. [14]. The peak distributions provide useful information of both the structure of the contact and that of the microscopic electrodes. It is suggested that the diverse excitations could be mapped in experiments by tuning the external dc voltage or the width of the leads.

9.6 Conclusions

Atomic-scale manipulation of materials leads to a richness of nanostructures with interesting, quantum-physics-dominated phenomena. The cohesive and electronic properties of nanowires can be explored by electronic structure calculations, which reveal the atomic geometry and intricate interplay between quantised electron states and their dynamics. The electron confinement dictates the conductivity, capacitance and the elongation force of metallic wires. Simple metal wires can become spontaneously spin-polarized at suitable wire radii.

Aknowledgements

We acknowledge the important contributions by our coworkers N. Zabala, C.C. Wan and Prof. Hong Guo.

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N	channel	surface(Ref. [10])
1	4.7 (2.5)	6.6 (2.0)
2	7.9 (1.6)	9.0 (1.4)
3	5.1 (2.5)	8.3 (1.6)
4	5.3 (2.4)	–

Table 3: Resistance (in KΩ) of a linear chain of Al atoms versus the chain length, N. In the parentheses, the conductance in units of of $G_0 = 2e^2/h$.

Figure Captions

Fig. 1. Surface energy (a), elongation force (b) and conductance for Na stabilized-jellium wires as a function of the wire radius (solid lines). In (a) the results of the extended liquid-drop model are also given by a dashed line [31]. When the wire radius increases the surface energy approaches that [31] for a planar stabilized-jellium surface. In (b) the forces derived from the surface energy of a planar surface ($-\pi R\sigma_{planar}$) are shown by a dashed line. The conductance in (c) is obtained from Eq. 1 by assuming $T_i(E_F) \equiv 1$. In (a) and (b) values corresponding to spin-polarized solutions are shown as black circles. In (c) unstable spin-compensated solutions are given with dashed lines.

Fig. 2. Stoner criterion product $I\tilde{D}$ for Na stabilized-jellium wires as a function of the wire radius. The regions of stable magnetic and spin-compensated solutions are denoted by filled and open markers, respectively.

Fig. 3. Band structure of a linear chain of Al atoms. The interatomic distance is the nearest-neighbor bulk distance of $d_{nn} = 5.41$ au. Majority and minority-spin bands calculated by the FLAPW method are shown by filled and open circles, respectively. They are compared with the corresponding stabilized-jellium-model results given solid and dashed lines.

Fig. 4. Total energy (a) and the magnetic moment per atom for a linear chain of Al atoms as a function of the interatomic distance. The results calculated by the FLAPW method for the spin-compensated and for the spin-polarized system are given by dashed and solid lines, respectively.

Fig. 5. The electrochemical capacitance C for the 5-atom tip-substrate system as a function of the distance d between the tip and the substrate: (a) classical and (b) quantum calculations. Details of the structure can be found in Ref. [14].

Fig. 6. Capacitances of the 5-atom tip junction. These systems are characterized by resonance transmission. Solid lines: $C(E)$ in units of 0.01aF. Dotted lines: $G(E)$ in units of $2e^2/h$. Dashed lines: the total reflection probability R.

Figures

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