DESIGN OF ATOMICALLY PRECISE NANOSCALE NEGATIVE DIFFERENTIAL RESISTANCE DEVICES

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EXECUTIVE SUMMARY

Downscaling device dimensions to the nanometer range raises significant challenges to traditional device design owing to potential current leakage across nanoscale dimensions and the need to maintain reproducibility while dealing with atomic-scale components. The research team has investigated negative differential resistance (NDR) devices based on atomically precise graphene nanoribbons. This computational evaluation of the traditional double-barrier resonant tunneling diode NDR structure uncovers important issues at the atomic scale concerning the need to minimize the tunneling current between the leads while achieving high peak current.

The team has proposed a new device structure consisting of multiple short segments that enables high current by the alignment of electronic levels across the segments while enlarging the tunneling distance between the leads. The proposed structure can be built with atomic precision using a scanning tunneling microscope (STM) tip during an intermediate stage in the synthesis of an armchair nanoribbon. In addition, the team has conducted an experimental evaluation of the band alignment at the interfaces and an STM image of the fabricated active part of the device.

RESEARCH CHALLENGE

Designing band alignment to manipulate electronic transport behaviors across an interface is the key to achieving novel functionalities in semiconductor junctions and heterostructures (HSs). The recent development of graphene and graphene nanoribbons (GNRs) offers new opportunities to design nanoscale devices and to test NDR at the atomic scale. Following the bottom-up synthesis of atomically precise GNRs, HSs based on GNRs with subnanometer widths and various types of band alignment were designed and fabricated. In particular, the controllable polymer-to-GNR conversion reaction was demonstrated using charge injection from an STM tip. This advance has enabled the creation of atomically precise HSs and devices based on single ribbons.

In the simplest resonant tunneling diode (RTD) configuration, a quantum dot is separated from the leads by barriers, leading to confined electron level(s). When the bias initially increases, the source Fermi level moves closer to the confined level, leading to a current increase. At a certain bias, resonant transmission is achieved, and the current reaches a maximum. As the bias increases further, the source Fermi level moves above the resonance and the current decreases. This results in an NDR region. When the bias increases further, the source Fermi level may approach another confined level and the current increases again. For an atomic-scale device, the conventional RTD design needs modification to become practical. First, the small size of the segments results in strong confinement, which limits the number of tunneling levels available at moderate voltages. Second, if the segments that are chosen are short, direct tunneling between leads may occur and thus wash out or eliminate the NDR. Conversely, if the segments are long enough to suppress direct tunneling, electron transmission across these regions with large electronic gaps results in a very small current, which may render the device impractical.

METHODS & CODES

The electronic structure calculations used the real-space multigrid (RMG) and plane-wave self-consistent field codes. The quantum transport nonequilibrium Green's function calculations used the localized orbitals and nonequilibrium Green's function branches of the RMG code.

RESULTS & IMPACT

In this work, the research team has demonstrated a practical device structure based on armchair GNRs to deliver a strong NDR effect. The proposed GNR-based HSs consist of seven-carbon-atom-wide armchair GNRs (7-aGNRs) and an intermediate structure appearing in GNR synthesis. This intermediate structure consists of partially converted GNRs with one side of the polyanthrylene converted to the GNR structure while the other side remains in the polymeric structure. The GNR/intermediate HSs have been confirmed to have a type-I band alignment, and thus can be employed to design NDR devices. After illustrating the key issues of NDR device design at the atomic scale, the team has proposed an unconventional multipart device comprised of five short segments, which leads to a pronounced NDR with a current large enough for practical use. Such a multipart HS can be experimentally fabricated by using *in situ* growth from polyanthrylene precursors and STM manipulations, ensuring an atomically precise device with well-defined, reproducible characteristics.

The team uses the GNR/intermediate junctions and undoped bulk graphene as paradigmatic probes and first considers the conventional quantum dot device model. In the simple GNR/intermediate/GNR double-barrier structure, two segments of the 7-aGNR, each with a length of four anthrylene units, approximately 17.0 Å, act as barriers, and they are directly connected to the bulk graphene leads. An intermediate structure of the same length, acting as a quantum dot, is sandwiched between the barriers, giving a structure labeled as a 4–4–4 HS. No obvious NDR is found, because direct tunneling can occur for this very short device. When much longer segments are used, NDR does occur, but the current decreases to the pA level, which is much too small to be used in devices.

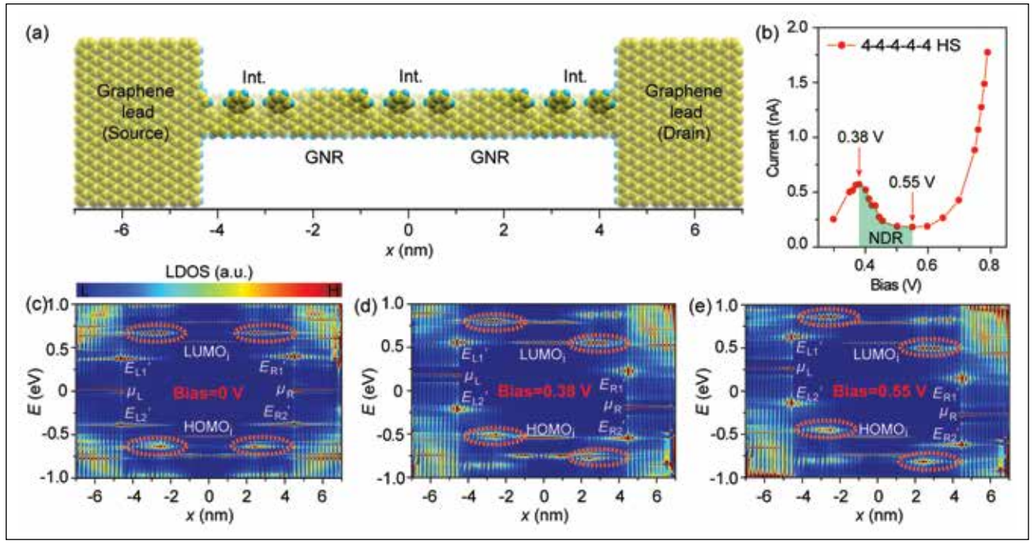

Figure 1: Atomic structure of a paradigmatic negative differential resistance (NDR) device consisting of three intermediate segments separated by two graphene nanoribbon segments. The NDR is marked with green shading. (c)–(e) Local density of states maps along the device showing alignment and misalignment of levels at zero bias, peak current, and current valley. (d) At 0.38 V bias, and (e) at 0.55 V bias. Note that the energy levels at −0.6 eV and 0.6 eV are aligned at the bias of 0.38 V and misaligned at 0.55 V. Dashed orange ellipses mark the states emerging between the graphene nanoribbon and outer intermediate segments.

To enlarge the magnitude of the current while enhancing the favorable NDR characteristics, the research team has proposed a new device design based on five short segments (Fig. 1). The team uses two 7-aGNR barriers and three intermediate parts, sandwiched between two graphene leads. Instead of connecting the 7-aGNR barriers directly to the graphene leads, the researchers inserted intermediate segments between the barriers and the leads to better align the energy levels on the opposite sides of the barriers. The use of five segments extends the active region of the device, preventing direct tunneling between the leads while allowing the barriers to be short, thereby enlarging the current. In the paradigmatic example, the team chose each segment to have the length of four anthrylene units, giving a 4–4–4–4–4 HS active region. In the calculated I–V curve in Fig. 1, the NDR appears at a relatively small bias with a large peak-to-valley ratio, which well satisfies the practical requirement for electronic circuit applications.

WHY BLUE WATERS

This application requires a very large parallel supercomputer with a high-speed interconnect between the nodes owing to the frequent exchange of substantial amounts of data between nodes. The evaluation and design of atomically precise structures required many runs to explore various scientific issues, with a substantial amount of analysis between the runs. High availability and quick turnaround are thus also very important for timely progress in this research.

PUBLICATIONS & DATA SETS

Z. Xiao *et al.*, "Design of atomically precise nanoscale negative differential resistance devices," *Adv. Theory Simul.*, vol. 2, p. 1800172, 2019, doi: 10.1002/adts.201800172.

C. Ma *et al.*, "Direct writing of heterostructures in single atomically precise graphene nanoribbons," *Phys. Rev. Materials*, vol. 3, p. 016001, 2019, doi: 10.1103/PhysRevMaterials.3.016001.