Spin-polarized Majorana zero modes in penta-silicene nanoribbons

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Majorana quasiparticles in condensed matter
Ramon Aguado, Rivista Del Nuovo Cimento 40, 523 (2017)

In search of Majorana
Sankar Das Sarma, Nature Physics, 19, 165 (2023)
SM/SC hybrids for topological superconductivity

**Excitation spectra in the trivial and topological regimes.** (a) Numerically calculated excitation spectra in the nanowire for (a) $V_z < V_c$ (where $V_c$ is the Zeeman splitting that corresponds to the TQPT) with no states in the superconducting), and (b) for $V_z > V_c$ showing localized MZMs at the wire ends. There are no states in the gap other than the two MZMs localized at the wire ends for $V_z > V_c$, whereas there are continuum metallic electron-hole excitations above the SC gap.
Majorana qubits for topological quantum computing

Ramón Aguado, and Leo P. Kouwenhoven, Physics Today 73, 6, 44 (2020)

FIGURE 1. (a) THE NANOWIRE PROPOSAL\(^3\) takes a nanowire of a semiconductor, such as indium arsenide or indium antimonide, that has strong spin–orbit coupling and places it in contact with an \(s\)-wave superconductor, such as aluminum, in the presence of an external magnetic field \(B\). As in the original model for one-dimensional \(p\)-wave superconductors,\(^4\) the nanowire device experiences a topological nontrivial phase with exponentially decaying Majorana bound states, denoted \(\gamma_L\) at both ends of the nanowire. (b) An actual device from Delft University of Technology includes various metallic gates for tuning it to the topological phase by adjusting the nanowire's chemical potential.

FIGURE 2. ANDREEV REFLECTIONS of electrons and holes to form Cooper pairs at the semiconducting–superconducting interface induce superconductivity in a nanowire. As a result, Majorana zero modes (flat red line) emerge in the energy spectrum as the external magnetic field increases. The Majoranas appear beyond some critical value of the external field (black dotted line) where the superconducting gap closes and reopens again, which signals a topological phase transition. Theory predicts that the emergent Majorana zero modes can be detected as a zero-bias anomaly in electrical conductance \(dl/dV\). (Image by R. Aguado and L. P. Kouwenhoven.)
Retraction Note: Quantized Majorana conductance

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Retraction to: Nature https://doi.org/10.1038/nature26142

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Detecting and distinguishing Majorana zero modes with the scanning tunnelling microscope
Berthold Jäck, Yonglong Xie, and Ali Yazdani, Nature Reviews Physics, 3, 541 (2021)

Key points

- Majorana zero modes (MZMs) are non-Abelian anyons that hold promise for facilitating topologically protected quantum computation. They can emerge as localized zero-energy states at the end of 1D topological superconductors.

- Scanning tunnelling microscopy (STM), with its ability to map the surface topography and probe the local electronic properties of samples with high spectral resolution, is particularly well suited to visualize MZMs on the atomic scale.

- STM experiments have demonstrated the presence of MZMs as localized end states of Fe chains on a Pb surface. Combining superconductivity with spin–orbit coupling and ferromagnetism, this model system realizes the Kitaev model for 1D topological superconductivity.

- High-resolution spectroscopy with the STM can explore various concepts for topological superconductivity and visualize the presence of localized zero-energy states across a plurality of material platforms, such as topological surface and boundary modes.

- Measurements using functional STM tips can probe other properties of zero-energy states, such as their spin signature. Through this capacity, these experiments are uniquely suited to distinguish topological from trivial zero-energy states.

- Future experiments with the STM on chains of magnetic atoms have the potential to demonstrate manipulation and braiding of MZMs, an important step towards realizing topologically protected quantum computation.
Box 1 | Visualizing Majorana zero modes with scanning tunnelling microscopy

The Kitaev model describes the hopping (with strength $t$) of spinless electrons between sites of a 1D chain in the presence of $p$-wave superconducting pairing, $\Delta_p$. Fractionalizing the fermionic modes into pairs of Majorana quasiparticles, the system can assume topologically distinct ground states: a topologically trivial state with on-site pairing (part a of the figure) and a topologically non-trivial state with nearest-neighbour pairing of Majorana quasiparticles (part b of the figure). Intuitively, in the topologically non-trivial case, two individual Majorana quasiparticles remain localized at the chain ends.

Material realization of the Kitaev model of 1D topological superconductivity can be achieved by considering the normal-state band structure of a 1D ferromagnet under the influence of Rashba spin-orbit coupling (SOC) with amplitude $E_{SO}$ (part c of the figure)\cite{11,47}. (a, lattice constant; $E$, energy; $k$, wave vector.) Ferromagnetic exchange splitting of strength $J$ separates minority and majority bands. When the Fermi level lies in the minority band, only one spin species is populated, and the system can be regarded as spinless. Rashba SOC imprints a momentum-dependent spin texture on these 1D states, which facilitates proximity-induced pairing by $s$-wave superconductor of the electrons in the otherwise fully spin-polarized minority band. This combination of magnetism and superconductivity therefore realizes a 1D topological superconducting state with $p$-wave pairing symmetry that can host zero-dimensional Majorana zero modes (MZMs) at its ends.

Scanning tunnelling microscopy (STM) experiments are ideally suited to study topological superconductivity and MZMs across nanoscopic material platforms (part d of the figure). In addition to the study of topographical sample properties\cite{100}, STM experiments can visualize localized MZMs at the ends of 1D topological superconductors, such as ferromagnetic chains of atoms placed on top of a superconducting surface\cite{24}. MZMs would appear as zero-energy states inside a superconducting gap in the measured conductance ($dI/dV$) spectrum of scanning tunnelling spectroscopy measurements. The use of functional tips diversifies the spectroscopic toolbox of STM measurements, aiding the measurement of electron-hole symmetry\cite{46} or spin signatures of MZMs\cite{46,47}, as discussed in the section on distinguishing trivial and topological zero-bias peaks.
From 2D to 1D silicon topological nanostructures
Silicene: Compelling Experimental Evidence for Graphenelike Two-Dimensional Silicon

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Archetype structure
3 × 3 reconstructed silicene
matching a 4 × 4 supercell on Ag(111)
Θ_{Si} = 18/16 = 1.125

Growth at 220 °C
LEED/STM

STM: The ‘Flower pattern’

Internal honeycomb arrangement unveiled only in 2017!

Only uncovered by near contact Atomic Force Microscopy
5 years later by Onoda et al., PRB 96, 241302(R) (2017)

WOS citations: 3093 on June 15, 2023

Initially refused by ‘Elite’ Journals without even sending the manuscript to referees!
Massively parallel silicon nanoribbons (SiNRs) grown on the Ag(110) surface (2004)

Nano-cultivation at RT, single strand SiNRs 8 Å in width

Nano-cultivation at 200°C 2 nm pitch
Nearly perfect array: ~ 5 \times 10^8 rows m⁻¹

Lavender field in Haute Provence
Ancestral cultivation: beauty and fragrance ~ 1 row m⁻¹

Serendipity!

0D Nanodots and 1D Nanoribbons,
single- or double-strand, i.e., 0.8 / 1.6 nm
in width grown at RT/200°C

Aligned, high aspect ratio, symmetry breaking
1D nanostructures!

Indication of superlubricity?

Nanodots, all identical, have mirror symmetry: Si₁₂ molecules

Salomon and Angot Science of Advanced Materials, 3 (2011) 1

The presence of 1D structures on the Ag(110) surface was inferred from tiny wiggles on the s region of the silver valence band noticed by chance at the Elettra facility in Trieste, Italy. The SiNRs were observed weeks later by STM.

a) Energy distribution curves for bare Ag(110) and for the dense array of SiNRs: Quantized states!
b) Band dispersion for the array of SiNRs vs kx along the Si NRs at ky = 0.7 Å⁻¹
c) and vs ky perpendicular to the Si NRs at kx = 0.35 Å⁻¹: Flat bands!

1D Dirac fermions

Yue et al., 22 (2022) 695

Edges states

Ronci et al., PSS C 11-12 (2010) 2710

ARPES measurements of the band structures. (a) Schematic drawing of the Brillouin zones of Ag(110) (black) and SiNRs (red). The blue lines indicate the five momentum cuts (Cuts 1–5) where (b–f) were taken. (b–f) ARPES intensity plots along Cuts 1–5 in (a). (g) Scheme of the TB model (a) Constant current 10×5 nm² STM image, V = +1.0 V, I = 10 nA, T = 80 K (b)-(h) Differential conductivity (dl/dV) images as a function of bias voltage. Marks are as a guide for better localizing the nanoribbons.
MZMs: Design Concept with pentasilicene NRs
**Inspiration**

Theoretical prediction of the possibility of obtaining spin-polarized Majorana Zero Modes at opposite edges of free standing double zigzag honeycomb nanoribbons, considering a tight-binding chain in a zHNR geometry.

Schematic of a zigzag honeycomb nanoribbon mimicking two parallel Kitaev chains connected by the hopping \( t \) (KzHNR). The equivalent B (A) atoms of the upper (lower) KzHNR are paired with each other via a p-wave superconducting parameter.

To properly break the spin degeneracy of the system, two additional effects in the spinless Hamiltonian \( H_t + H_\Delta \) are introduced: the extrinsic Rashba spin-orbit coupling (RSOC) and an external magnetic field (EMF). The extrinsic RSOC lifts the corresponding bands’ spin degeneracy, unless at \( k = 0 \). Additionally, the EMF applied perpendicularly to the ribbon plane drives the system through topological phase transitions (TPTs) exhibiting spin-polarized MZMs. In this situation, spin-discriminated MZMs emerge at the ends of the double-spin KzHNR structure. The corresponding generalized Hamiltonian is given by

\[
H_{\text{total}} = H_t + H_\Delta + H_R + H_Z
\]

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**Spin-polarized Majorana zero modes in double zigzag honeycomb nanoribbons**

The Hardware

Perfectly clean, atomically thin and precise, massively parallel single strand penta-silicene nanoribbons, 0.8 nm in width and several hundred nanometers in length, grown in situ under UHV on a Ag(110) surface.

(a) and (b) Experimental STM images (uncorrected drift, courtesy Eric Salomon, PIIM Marseille).
(c) Highresolution nc-AFM image.
(d) Top and cross view of the arrangement of the Si pentagonal building blocks.
(e) Confirmation of the presence of a Dirac cone.

(c) Sheng et al., Nano Lett. 2018, 18, 2937
(d) Cerda et al., Nature Comm., 7 (2016) 13076
(e) Yue et al., Nano Lett. 2022, 22, 695
Emergence of spin-polarized Majorana zero modes in penta-silicene nanoribbons

The calculations:
- to simplify we choose right angle chains with all hoppings (first neighbors) equal to \( t' \)
- Rashba spin-orbit interaction \( \lambda_R \)
- External magnetic field \( E_z \) perpendicular to the NR plane, introducing a Zeeman effect, to properly account for the spin degree of freedom in the superconducting p-SiNR.
- Superconductor p-wave pairing \( \Delta \)

The total system Hamiltonian, considering also the spin degree of freedom on both \( H_t \) and \( H_\Delta \) is defined as \( H_{\text{total}} = H_t + H_Z + H_R + H_\Delta \)

The realization:
since silver is not a superconductor, to generate a p-wave pairing \( \Delta \) on the pink atoms of (c), we overlay \textit{in situ} a thin unreactive lead film evaporated through a mask. Under the presence of a strong RSOC coming from the Pb atoms and an applied magnetic field, the s-wave Cooper pairs of the Pb film can enter into the p-SiNR region via proximity effect, giving rise to a p-wave-induced pairing in the double chain structure.
Results for p-SiNRs

**Spinless case**

(a)-(c) Bulk energy dispersion for the spinless p-SiNRs as a function of \( k_x \), for \( \mu = 0.0t, 0.4t, \) and \( 0.7t \), respectively. (d) Energy spectrum as a function of the chemical potential. Vertical lines indicate the chosen values of chemical potential shown on top panels. (e)-(g) The energy spectrum with labels the energy levels in increasing order for \( \mu = 0.0t, 0.4t, \) and \( 0.7t \), respectively. (i)-(k) Probability density associated with zero-energy states, as a function of the lattice site \( N = 1 \ldots 100 \).

**Spinfull case**

See the manuscript...

**Take home message**

The MZMs are spin discriminated, and their polarization can be controlled by varying the chemical potential or the magnetic field.

Hence, the p-SiNRs appear as candidates for realizing topological qubits based on MZMs with well-defined spin orientation, suggesting a possible route for performing Majorana spintronics.
The Mantra

Without deviation from the norm, progress is not possible.

—Frank Zappa
Lifting off double-strand SiNRs with an STM tip

R. Hiraoka et al., Beilstein J. Nanotechnol. 2017, 8, 1699
From the group of Prof. Maki Kawai

Free-standing pentasilicenelike nanoribbon!

“I don’t often say something categorical, but I will say that a pristine free-standing single layer sheet of silicene (or a Si nanotube) will not be made.” R. Hoffmann Angew. Chem. Int. Ed. 52, 93 (2013).

Open Questions:
Why symmetry-breaking Single Strand SiNRs develop on a Ag missing row from symmetric NanoDots on a Ag divacancy? What is the polymerisation process?
How Single Strand SiNRs, which form a $3 \times 2$ arrangement, evolve to Double Strand SiNRs and form the highly perfect $5 \times 2$ grating? Lateral compaction? Superlubricity?
(a) STM image of an ensemble of multilayer-thick SiNRs on Ag(110) (400×400 nm²; V=-0.6 V; I=1 nA); (b) STM 3D enlarged view of (30×20 nm²; V=0.2 V; I=0.1 nA); (c) P1 line profile along the [100] Ag direction: pyramidal cross section

De Padova et al., Nano Letters, 12 5500 (2012)
Dirac fermions in multilayer-thick SiNRs

(a) ARPES intensities ($h\nu = 126$ eV) from multilayer-thick $5\times4$ SiNRs recorded along their lengths the ($\Gamma \rightarrow X$) direction; (b) zoom-in; (c) vertical cut along the blue arrow in (b)

De Padova et al., Nano Letters, 12 5500 (2012)
Massively parallel, high aspect ratio, Germanium NRs prepared by surface segregation on a Ag(110) thin film grown on a Ge(110) surface

(a) Large-scale STM (b) Atomic scale STM image. (c) Zoomed-up STM image. (d) Section profiles along white lines in (a). (e) LEED pattern at 55 eV. White solid circles are primitive spots of Ag(110). Green solid circles are incommensurate spots of c(4 × 2.8) and yellow solid circles are multiple diffraction spots originating from (01), (10), (0-1), and (-10). (f) FFT image of (b). (g) Scheme of the incommensurate Ag(110)c(4 × 2.8) supercell.

The Ag(110) thin film was grown on a Ge(110) substrate and annealed at 510°C

Yuhara et al., AppL Surf. Sci., 550 (2021) 149236
(a) Left: Spatial variation of the superconducting gap crossing the A edge along the dotted arrow in the image of the island (right). The contour map is projected underneath.

(b) Plots of the gaps ($\Delta$) extracted by half the energy distance of two coherence peaks and the zero bias conductance (ZBC) that quantizes the degree of the superconducting gap compared with a full gap.
When a Topological insulator is coated by an s-wave superconductor, the superconducting vortices are Majorana fermions—they are their own antiparticles. Exchanging or braiding Majorana vortices leads to non-abelian statistics. Such behavior could form the basis piece of hardware (Majorana Qubit) for topological quantum computing. Experimental synthesis and characterization of 2D Topological Insulators remain a major challenge at present, offering outstanding opportunities for innovation and breakthrough. Kou et al., J. Phys. Chem. Lett. 2017, 8, 1905

The way: create atomically controlled artificial structure by design

Nanoarchitectonics!

The concept by Prof. Masakazu Aono
MANA, NIMS, Japon

Sir Roger Penrose, 2020 Nobel Prize in Physics.