Recreating Cuprate Physics on a Silicon Platform

Hanno H. Weitering

University of Tennessee

What it takes to be super…

- Dissipationless electrical conductivity below $T_c$
- Perfect diamagnetism below $T_c$ (Anderson-Higgs mechanism for ‘massive photons’)
Formation of a Cooper pair condensate

\[ \Delta_0 = 2\hbar\omega_D e^{\frac{-1}{V_0D(E_F)}} \]

- Fermi sphere
- Superconducting gap

credit P. Hirschfeld
Superconducting Quantum Devices

DC: \( J = J_0 \sin(\theta_1 - \theta_2) \)

AC: \( \langle J(t) \rangle = J_c \sin[\theta(0) + \omega t] \quad \omega = \frac{2e}{\hbar} V \)

\( \hbar \omega = 2eV \)

1 mV \( \cong \) 484 MHz

‘The study of superconductivity is littered with disappointments, dead ends, and serendipitous discoveries’*

*Prof. Antia Botana, ASU
Outline

• Background & overview

• **Recreating cuprate physics**: Triangular tin lattice on a silicon template

• Modulation doping and evidence for Mott physics

• Superconducting properties

• Time reversal symmetry breaking and d-wave pairing

• Conclusions and outlook

• Electron doping and charge ordering
• Doped Mott insulators
• Quasi 2D phenomenon

Keimer et al. Nature ‘15
a dream.....
**Mott Physics 101**

- **vacuum level**

- **atomic limit**

- **Insulator – metal (Mott) transition when** $U^* \cong W$

- **IE**

- **EA**

- **U**

- **U**

- **W**

- **DOS**

- **condensed matter**

- **crystal**
Doping a Mott Insulator

Frustration: spin pairs cannot all be simultaneously in the lowest energy configuration.

\[ \hat{H} = \frac{1}{2} \sum_{i,j} J_{ij} \hat{S}_i \hat{S}_j \]

\[ J_{ij} = \frac{4t_{ij}^2}{U} \]
2D quantum spin liquid versus classical Neel order

Classical Neel long-range order (120°) for large U/W

RVB: frustration, low spin, low dimensionality

Metallization or doping: route to high Tc superconductivity?
Order parameter symmetry

\[ \Psi = \Delta_0 e^{i\phi} \]

conventional
Sn, Pb, MgB\textsubscript{2}…
phonon mediated

unconventional
high-Tc cuprates
strong Coulomb repulsion

\[ \Delta_k = -\frac{1}{N} \sum_{k'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}} \tanh \left( \frac{E_{k'}}{2k_B T} \right) \]
‘Exotic’ chiral d-wave order parameter

- triangular lattice
- $d_{xy}$ and $d_{x^2-y^2}$ order parameters 90° out of phase
- broken TRS

- topology set by Chern/winding number of order parameter
- $d+id$ wave winds twice around $\Gamma$ ($N = 2$)
- 2 chiral copropagating edge states per edge

- $Na_xCoO_2 \cdot yH_2O$, hole-doped graphene, SrPtAs,........

A.M. Black-Schaffer et al., JPCM 26, 423201 (2014)
Submonolayer of Sn on Si(111)

$(\sqrt{3} \times \sqrt{3})$ superlattice at 1/3 monolayer of Sn

Single-band Mott insulator ($T < 100$ K)

Close realization of a spin $\frac{1}{2}$ triangular lattice antiferromagnetic Heisenberg system

Potential for chiral superconductivity with doping ($\Delta_1 \pm i\Delta_2$)
Competing phases

- 3x3 charge ordered metal
- 3x3 charge ordered insulator

E.g., Sn on Ge(111) or Pb on Si(111) or Ge(111)


R. Cortes et al, PRB 88, 125113 (2013)
Magnetic order in a frustrated two-dimensional atom lattice at a semiconductor surface

Gang Li¹, Philipp Höpfner², Jörg Schäfer², Christian Blumenstein², Sebastian Meyer², Aaron Bostwick³, Eli Rotenberg³, Ralph Claessen² & Werner Hanke¹

DFT

DFT+DCA

ARTICLE
Received 26 Oct 2012 | Accepted 20 Feb 2013 | Published 27 Mar 2013
DOI: 10.1038/ncomms2617

a) ΓK
b) LDA+DCA

ARPES

\[ E_{\text{F}} \]

\[ E_{\text{F}} \]

\[ E_{\text{F}} \]

\[ E_{\text{F}} \]
Magnetic order in a frustrated two-dimensional atom lattice at a semiconductor surface

Gang Li¹, Philipp Höpfner², Jörg Schäfer², Christian Blumenstein², Sebastian Meyer², Aaron Bostwick³, Eli Rotenberg³, Ralph Claessen² & Werner Hanke¹

Sn/Si(111)
Why is this system interesting: direct access to Mottness!

Cuprates, Complex oxides

Scanning Tunneling Microscopy and Spectroscopy

STM

QPI

STS

dl/dV \propto LDOS
Doping the Sn terminated Si(111) surface

Modulation Doping Scheme

Heavily B-doped (p-type) Si substrates

Ming et al., PRL 119, 266802 (2017)
Doped Mott insulator, spectral weight transfer and van Hove singularity

$U \approx 0.6 - 0.7$ eV

$W \approx 0.6$ eV

10% hole doping ($p = 0.1$)

Ming et al., PRL 199, 266802 (2017)
Quasi Particle Interference Imaging Sn on Si(111)

Ming et al., PRL 199, 266802 (2017)
Fermi surface

QPI

T-matrix simulation

DFT
Superconductivity

Wu et al., PRL 125, 117001 (2020)

\[ p = 0.1 \]
Superconductivity

$p = 0.1$

$T_c = 4.7 \pm 0.3 \text{ K}$

$T_c$ similar to that of $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$

Vortices

\[ p = 0.1 \]

\[ H_{c2}(0 \text{ K}) = 3 \text{ T} \]

\[ T_c = 4.7 \pm 0.3 \text{ K} \]

Wu et al, PRL 125, 117001 (2020)
Doping dependence

$p = 0.08$

$T_c = 7.6 \pm 0.2 \text{ K}$

$s$ wave:

- $\Delta_0 = 2.16 \text{ mV}$,
- $T_c = 7.8 \text{ K}$

$d + id$ wave:

- $\Delta_0 = 0.50 \text{ mV}$,
- $T_c = 7.4 \text{ K}$

Normalized $dl/dV$ (arb. u.)

bias (mV)

Extracted $\Delta_0$ (mV)

Temperature (K)
Doping dependence

$p = 0.08$

$B_c \approx 13$ T

$T_c \approx 7.7$ K

$T_c \approx 9$ K

$p = 0.08$

$p = 0.08$

$p = 0.06$

$p = 0.06$
Fitting the superconducting gap

Chiral d-wave versus (anisotropic) s-wave
Central ‘flower’ feature from time-reversal symmetry breaking due to

magnetic defect scattering \textit{versus} chiral order parameter (e.g. $d_{x^2-y^2} \pm id_{xy}$)
Defect scattering

\[ V = \text{adatom vacancy} \]
\[ S = \text{substitutional Si atom} \]
\[ A = \text{extra Sn adatoms} \]
\[ O_n (1-6) = \text{unknown defects} \]

All types of defect produce a pair of gap states. Either they are all magnetic or the superconductor breaks time-reversal symmetry (as in \(d+id\) or \(p+ip\)).
Magnetic defects?

Simulations by Cesar Gonzalez and Jose Ortega (Madrid)

**Sn adatom defect**

**Experiment**

**Simulation**

**Substitutional defect**

Spin-polarized DFT indicates that defects are non-magnetic.

Good agreement between experimental and simulated STM images from DFT gives confidence that the DFT results are correct.

Chiral order parameter most likely interpretation (d+id or p+ip).

p+ip ruled out.

Simulations by Cesar Gonzalez and Jose Ortega (Madrid)
Near-edge ZBC in STM is consistent with existence of chiral edge states

J. Strockoz and J. Venderbos (Drexel)
Conclusions and Outlook

• 1/3 ML of Sn transforms a hole-doped Si(111) semiconductor surface into a superconductor. Exceptionally clean and simple materials system

• Evidence points to Mott physics and chiral d-wave pairing

• Consistent with theoretical predictions for Sn/Si(111), e.g., Cao et al., PRB 97, 155145 (2018) and Wolf et al., PRL 128, 167002 (2022), as well as our own DCA results

• Semiconductor surfaces may be ideal test bed for studying and exploiting correlated topological states of matter

• Superconductor can possibly be altered or engineered using standard semiconductor processing or surface science approaches
Electron doping via K deposition

T.S. Smith et al, PRL 124, 097602 (2020)
(2√3×2√3)R30° charge-ordered insulator

-1.5 V
Sn ‘up’

+2.5 V
K adatoms

+1.0 V
Sn ‘down’

PRL 124, 097602 (2020)
50% electron doping: Charge order $T^* \sim 290$ K
PRL 124, 097602 (2020)

Zero doping: Mott insulator
PRL 119, 266802, (2017)

6~8% hole doping:
Superconductivity $T_c \approx 7$~9 K

10% hole doping:
Superconductivity $T_c \sim 4.5$ K
PRL 125, 117001 (2020)
THANK YOU
Structure of the Cooper pair

**Real Space Picture**

\[ \Delta_{ij} = \Delta_{ln} e^{i\theta_{ij}} \]

\[ \theta_{i,j} = \vec{r}_{ij} \cdot \hat{x}, \quad \vec{r}_{ij} = \vec{r}_i - \vec{r}_j \]

\[ l = 2, \; n = 1 \]

Structure of the Cooper pair

Real Space Picture

$$\Delta_{ij} = \Delta_{ln} e^{i\theta_{ij}}$$

$$\theta_{i,j} = \vec{r}_{ij} \cdot \hat{x}, \quad \vec{r}_{ij} = \vec{r}_i - \vec{r}_j$$

$$l = 2, n = 1$$


Momentum Space Picture

$$\Delta_{ln}(k) = 2 \left[ \beta'_{ln}(k) + i \beta''_{ln}(k) \right]$$

Chiral \(d\)-wave pairing (\(\ell = 2\))

<table>
<thead>
<tr>
<th>(n)</th>
<th>(\beta'_{2n}(k))</th>
<th>(\beta''_{2n}(k))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(\cos k_x - \cos \frac{\sqrt{3}}{2} k_y \cos \frac{\sqrt{3}}{2} k_y)</td>
<td>(\sqrt{3} \sin \frac{\sqrt{3}}{2} k_x \sin \frac{\sqrt{3}}{2} k_y)</td>
</tr>
<tr>
<td>2</td>
<td>(\cos \sqrt{3} k_x - \cos \frac{\sqrt{3}}{2} k_y \cos \frac{\sqrt{3}}{2} k_x)</td>
<td>(-\sqrt{3} \sin \frac{\sqrt{3}}{2} k_y \sin \frac{\sqrt{3}}{2} k_x)</td>
</tr>
<tr>
<td>3</td>
<td>(\cos 2k_y - \cos \sqrt{3} k_x \cos k_y)</td>
<td>(\sqrt{3} \sin \sqrt{3} k_x \sin k_y)</td>
</tr>
</tbody>
</table>

*Note: Zhou & Wang’s \((k_x,k_y)\) is rotated 90 degrees relative to my real space picture.*
Competing explanations

- States at the Fermi level are related to a boron impurity band

\[ \text{Coherent QPI scattering produces Fermi surface of } (\sqrt{3} \times \sqrt{3}) \text{ Sn adatom reconstruction} \]

- Gap states are conventional YSR states associated with magnetic defects in an s-wave superconductor

\[ \text{One would have to assume that all defects, including the extra Sn adatoms and substitutional Si atoms are magnetic. DFT results are in excellent agreement with the STM data of substitutional and Sn adatom defects, and thus likely correct} \]

- Edge states are merely the result of an inverse proximity effect.

\[ \text{Possibly true. More investigations are needed.} \]

- Pairing symmetry is p+ip or higher angular momentum pairing channels

\[ \text{Gap fitting doesn’t work for p-wave. DCA calculations indicate d+id is the leading pairing instability} \]
Topography (-2 V)

Topography (20 mV)

$\xi = 5.1 \pm 0.5 \text{nm}$

$\xi = 4.9 \pm 0.3 \text{nm}$