Phase separation at the dimer-superconductor transition in $\text{Ir}_{1-x}\text{Rh}_x \text{Te}_2$

*a tale of a negative result*

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IrTe$_2$: properties

- **HT structure** trigonal $P\overline{3}m1$
- Interlayer spacing smaller than the van der Waals gap
- Ir$^3+$Te$_2^{1.5}$-like, covalent Te-Te
- Pauli paramagnetic metallic

$P\overline{3}m1$
IrTe$_2$: dimerization = large distortions

1) Dimer contraction $\Delta r=0.83$ Å

2) Only $\sim$6% of Ir-Ir bonds are dimerized

G.L. Pascut et al., PRL (2014)
Substitution/intercalation suppresses LT phase and SC appears

- Reminiscent of unconventional SCs
- Looks like a tunable competition at play

• What is the origin of the LT phase in IrTe₂?
• LT phase competes with SC in a QCP–manner?
• Fluctuations involved in the SC mechanism?
IrTe$_2$: local fluctuating Ir dimers survive at high temperature?!

**Ir L3-edge EXAFS**

B. Joseph et al., PRB (2013)

1) Te-dimers and Ir-Te regularize at high-T
2) Ir-dimers survive locally at high-T
3) Transition has order-disorder character

- Interpretation based on C2/m-model
- Early model of LT phase is **wrong**
- This is not really happening!
Samples studied: IrTe$_2$, Ir$_{1-x}$Rh$_x$Te$_2$ (0<x<0.3), Ir$_{0.95}$Pt$_{0.05}$Te$_2$

- Reminiscent of unconventional SCs
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- What is the origin of the LT phase in IrTe$_2$?
- LT phase competes with SC in a QCP-manner?
- Dimer fluctuations involved in the SC mechanism?
Experiment: x-ray atomic Pair Distribution Function 10K-300K

IrTe$_2$, Ir$_{1-x}$Rh$_x$Te$_2$ (0<x<0.3), Ir$_{0.95}$Pt$_{0.05}$Te$_2$
Detectability of IrTe$_2$ dimers by PDF

- Dimer associated distortions clearly seen in PDF
  \[ \Delta r(\text{Ir-Ir}) = -0.8\,\text{Å (dimer)} \]
  \[ \Delta r(\text{Te-Te}) = -0.5\,\text{Å (dimer)} \]
  \[ \Delta r(\text{Te-Te}) = +0.3\,\text{Å (lateral)} \]

- Dimers **disappear** locally in the high temperature metallic phase in disagreement with EXAFS

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**trigonal**

**triclinic**

**300K**

**220K**
Properties of the samples studied
Changes with temperature

Diffraction
- Long range dimer order in IrTe$_2$
- No long range order for SC compositions

PDF
- Short range structure changes in IrTe$_2$
- For SC compositions changes dominantly of thermal origin
Data morphing (x & y scaling)

- IrTe$_2$ 300K and 10K data cannot be morphed one onto another
- 5% Pt & 20% Rh data morphable
- For SC compositions changes dominantly thermal in origin
Trigonal high-T model fits

- Fits well IrTe$_2$ data at 300K
- Fails for IrTe$_2$ data at 10K
- Fits well 5% Pt data at 10K
- Fits well 20% Rh data at 10K
Trigonal model fit results vs temperature

- Upturn in ADPs at the onset $T$ of long range ordered dimers ($\text{IrTe}_2$)
- Upturn in Ir-ADPs at the onset $T$ of local fluctuating dimers (Cr-doped CuIr$_2$S$_4$ spinel)
- No upturn in 5% Pt and 20% Rh substituted IrTe2 down to 10 K
- Sensitivity to $\sim$0.5% of dimerized Ir-Ir
Sensitivity of ADP to the presence of dimers

(a) PDF, $G(\AA^{-2})$

(b) $U_{iso} \times 100 (\AA^2)$

interatomic distance, $r (\AA)$

fraction of dimerized Ir-Ir bonds (%)
Changes with Rh-substitution and temperature

- Long range dimer order in IrTe₂
- Long range order fading out toward SC Rh-compositions

Diffraction

\( \text{Ir}_{1-x}\text{Rh}_x\text{Te}_2 \)

300K

10K
Changes with Rh-substitution and temperature

PDF
- At 300K all PDFs similar
- At 10K PDFs cluster in two groups

Ir\textsubscript{1-x}Rh\textsubscript{x}Te\textsubscript{2}

At 300K all PDFs similar
At 10K PDFs cluster in two groups
Low temperature behavior

Superconductivity

Local structure

Ir$_{1-x}$Rh$_x$Te$_2$
Structural behavior at 10K

P$_3$m$_1$ dimer-free model

$P\Gamma$ dimerized structure model

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Phase separation in $\text{Ir}_{1-x}\text{Rh}_x\text{Te}_2$ ($0<x<0.3$)

- Dimer-related disorder weakens as Rh-content increases
- Phase separation close to dimer/SC boundary
- Transition between dimer/SC seems to be weakly first-order

Static dimer density & sharpness of the dimer/SC transition

- $T_S$ linear in $x$
- Sudden drop at dimer/SC boundary
- Similarly, sharp rise with pressure

From dip in susceptibility
- Gradual depletion with $x$
- Vanishes for SC compositions

Summary

• No evidence for fluctuations of the dimer phase in the SC range of compositions
• No evidence for fluctuating local dimers in the HT phase of IrTe$_2$
• Phase separation close to dimer/SC boundary at 10K
• Dimer/SC transition weakly first order
• Fluctuating dimers not relevant aspect of the phase diagrams of IrTe$_2$
• QCP-scenario for dimer/SC interplay implausible
