Course Outline

Monday	Tuesday	Wednesday	Thursday	Friday
Lecture 1 10-10h45 Marc	**Lecture 4** 10-10h45 Thomas	**Lecture 7** 10-10h45 Thomas	**Lecture 10** 10-10h45 Marc	**Lecture 13** 10-10h45 Johan
Lecture 2 11-11h45 Johan	**Lunch - Mensa**	**Lecture 8** 11-11h45 Marc	**Lecture 11** 11-11h45 Marc	**Lecture 14** 11-11h45 Johan
Lunch - Mensa	**Lecture 5** 13-13h45 Thomas	**Lunch - Mensa**	**Lunch - Mensa**	**Lunch - Mensa**
Lecture 3 13h30-14h15 Thomas	**Lecture 6** 14-14h45 Thomas	**Lecture 9** 13h30-14h15 Marc	**Lecture 12** 13-14h15 Johan	**Lecture 15** 13-14h15 Johan
		Exercise Class 14h30-16		Exercise Class 14h30-16

- Introduction & overview. Why is scattering experiments important? (green)
- Theoretical background for scattering experiments (orange)
- Scattering on condensed matter systems + Neutron scattering experiments (blue)
- X-ray diffraction and spectroscopy techniques (purple)

X-ray Scattering Methodology

	Diffraction	Spectroscopy
Resonant	**REXS & XAS** Site sensitivity Charge ordering	**RIXS & XAS** Spin excitations Orbital excitations
Non-Resonant	**XRD** Crystal structure Charge-density-wave Extreme environments	**IXS** Phonons dispersions Kohn anomalies

Outline

IXS
Phonons dispersions
Kohn anomalies

XAS
Site sensitivity
Charge ordering

XRD
Crystal structure
Charge-density-wave
Extreme environments

Neutron Scattering
Magnetism
Heavy Fermion Physics

Time – Independent Scattering Theory

Scattering Amplitude $\langle f|V|i\rangle$

REXS & RIXS
Spin excitations
Orbital excitations

RMP **83**, 705 (2011)

Time – Dependent Scattering Theory

$$\mathcal{F}_{fg}(\mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}', \omega_{\mathbf{k}}, \omega_{\mathbf{k}'}) = \sum_n \frac{\langle f|\mathcal{D}'^{\dagger}|n\rangle\langle n|\mathcal{D}|g\rangle}{E_g + \hbar\omega_{\mathbf{k}} - E_n + i\Gamma_n}$$

Retraction Note: Room-temperature superconductivity in a carbonaceous sulfur hydride

Elliot Snider, Nathan Dasenbrock-Gammon, Raymond McBride, Mathew Debessai, Hiranya Vindana, Kevin Vencatasamy, Keith V. Lawler, Ashkan Salamat & Ranga P. Dias

Nature **610**, 804 (2022) | Cite this article

The Original Article was published on 14 October 2020

This article has been updated

Retraction to: *Nature* https://doi.org/10.1038/s41586-020-2801-z Published online 14 October 2020

The editors of *Nature* wish to retract this paper. Following publication, questions were raised regarding the manner in which the data in this paper have been processed and analysed, which the authors and *Nature* have been working to resolve.

We have now established that some key data processing steps—namely, the background subtractions applied to the raw data used to generate the magnetic susceptibility plots in Fig. 2a and Extended Data Fig. 7d—used a non-standard, user-defined procedure. The details of

Crystal structure of the superconducting phase of sulfur hydride

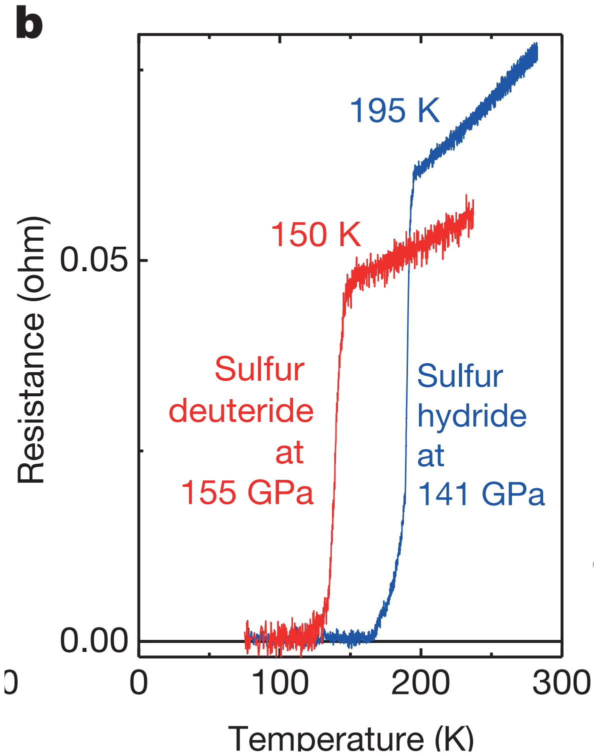
Nat. Phys. 12, 835 (2016)

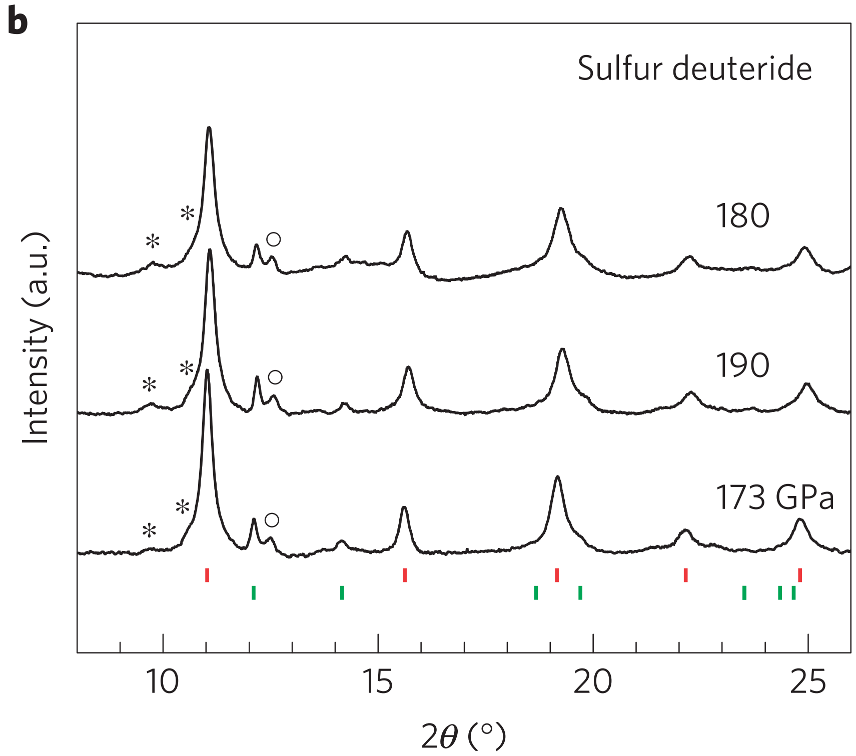
Mari Einaga[1*†], Masafumi Sakata[1], Takahiro Ishikawa[1], Katsuya Shimizu[1†], Mikhail I. Eremets[2†], Alexander P. Drozdov[2], Ivan A. Troyan[2], Naohisa Hirao[3] and Yasuo Ohishi[3]

Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system

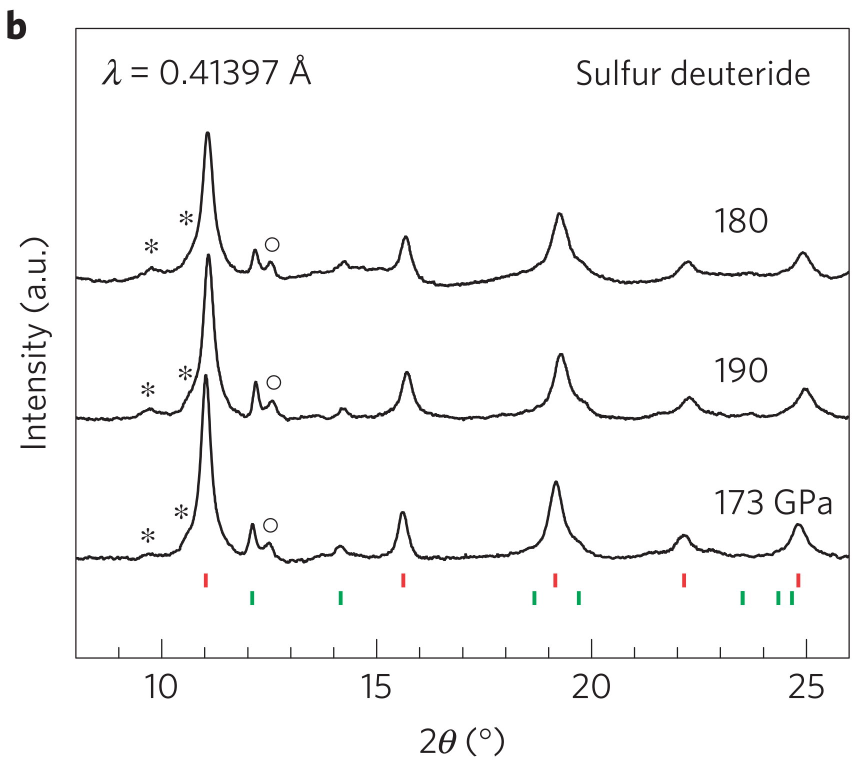
Nature 73, 525 (2015)

A. P. Drozdov[1*], M. I. Eremets[1*], I. A. Troyan[1], V. Ksenofontov[2] & S. I. Shylin[2]





Peak Number (PN)	2θ (Degrees)	$\frac{\mathrm{Sin}[\theta(\mathrm{PN})]}{\mathrm{Sin}[\theta\ (\mathrm{PN}=1)]}$	$\frac{d(1)}{d(PN)}[BCC]$	$\frac{d(1)}{d(PN)}[FCC]$
1	11	1		
2	15.7	1.4		
3	19.2	1.7		
4	22.1	2		
5	24.9	2.25		



$$S_{BCC} = \begin{cases} 2f, & h+k+l = \text{even} \\ 0, & h+k+l = \text{odd} \end{cases} \qquad S_{FCC} = \begin{cases} 4f, & h,k,l \text{ all even or all odd} \\ 0, & h,k,l \text{ mixed even/odd} \end{cases}$$

Table 1: The plane distance d = $2\pi/\sqrt{h^2+k^2+l^2}$ for different Miller indices (hkl) and the structure factor S for different structures.

Index i	(hkl)	d (2π)	S_{BCC}	S_{FCC}	
1	(100)	1			
2	(110)	$1/\sqrt{2}$			
3	(111)	$1/\sqrt{3}$			
4	(200)	1/2			
5	(210)	$1/\sqrt{5}$			
6	(211)	$1/\sqrt{6}$			
7	(220)	$1/\sqrt{8}$			
8	(221)	$1/3$			
9	(300)	1/3			
10	(310)	$1/\sqrt{10}$			
11	(311)	$1/\sqrt{11}$			
12	(400)	1/4			

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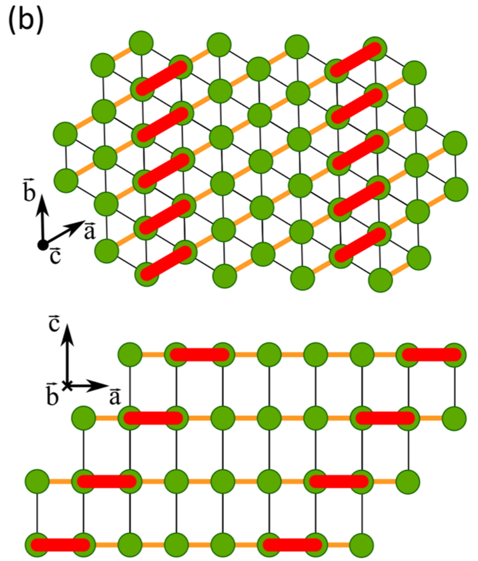
Index i	(hkl)	d (2π)	S_{BCC}	S_{FCC}	
1	(100)	1	= 0	= 0	
2	(110)	$1/\sqrt{2}$	$\neq 0$	= 0	
3	(111)	$1/\sqrt{3}$	= 0	$\neq 0$	
4	(200)	1/2	$\neq 0$	$\neq 0$	
5	(210)	$1/\sqrt{5}$	= 0	= 0	
6	(211)	$1/\sqrt{6}$	$\neq 0$	= 0	
7	(220)	$1/\sqrt{8}$	$\neq 0$	$\neq 0$	
8	(221)	$1/3$	= 0	= 0	
9	(300)	1/3	= 0	= 0	
10	(310)	$1/\sqrt{10}$	$\neq 0$	= 0	
11	(311)	$1/\sqrt{11}$	= 0	$\neq 0$	
12	(400)	1/4	$\neq 0$	$\neq 0$	

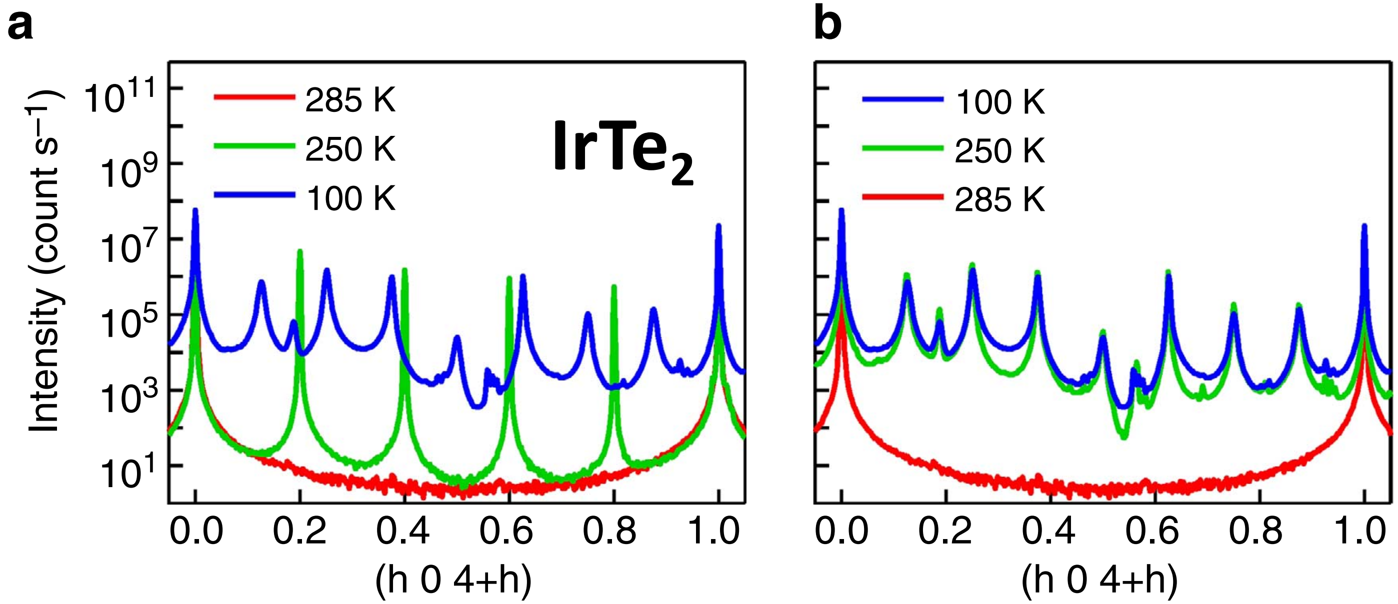
Peak Number (PN)	2θ **(Degrees)**	$\frac{\mathrm{Sin}[\theta(\mathrm{PN})]}{\mathrm{Sin}[\theta\ (\mathrm{PN}=1)]}$	$\frac{d(1)}{d(PN)}[BCC]$	$\frac{d(1)}{d(PN)}[FCC]$
1	11	1	1	1
2	15.7	1.4	1.41	2/sqrt(3) = 1.15
3	19.2	1.7	sqrt(3)=1.73	sqrt(8/3)=1.6
4	22.1	2	2	sqrt(11/3)=1.9
5	24.9	2.25	sqrt(5)=2.24	4/sqrt(3)=2.31

Charge-ordering cascade with spin-orbit Mott dimer states in metallic iridium ditelluride

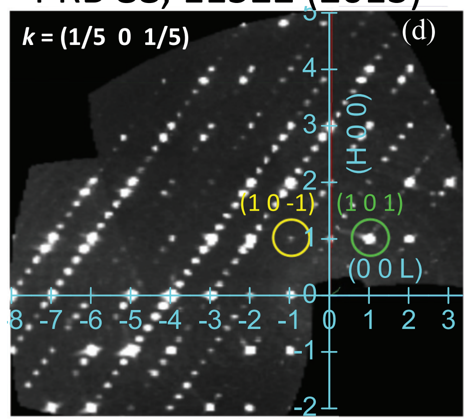
K.-T. Ko[1,2,3], H.-H. Lee[1,2], D.-H. Kim[1,2], J.-J. Yang[2,4], S.-W. Cheong[4,5], M.J. Eom[6], J.S. Kim[6], R. Gammag[6], K.-S. Kim[6], H.-S. Kim[6,7], T.-H. Kim[6,7], H.-W. Yeom[6,7], T.-Y. Koo[8], H.-D. Kim[8,9] & J.-H. Park[1,2,10]

NATURE COMMUNICATIONS | 6:7342 | DOI: 10.1038/ncomms8342 |





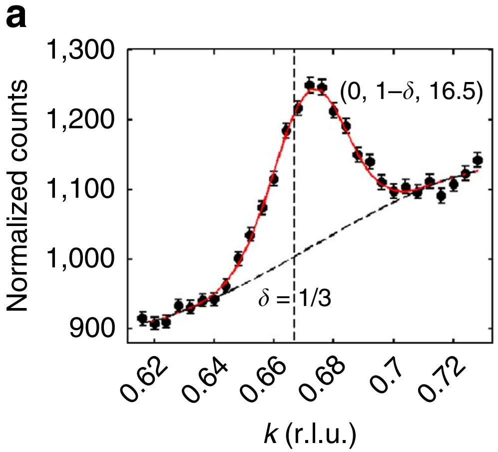
PRB **88**, 11522 (2013)

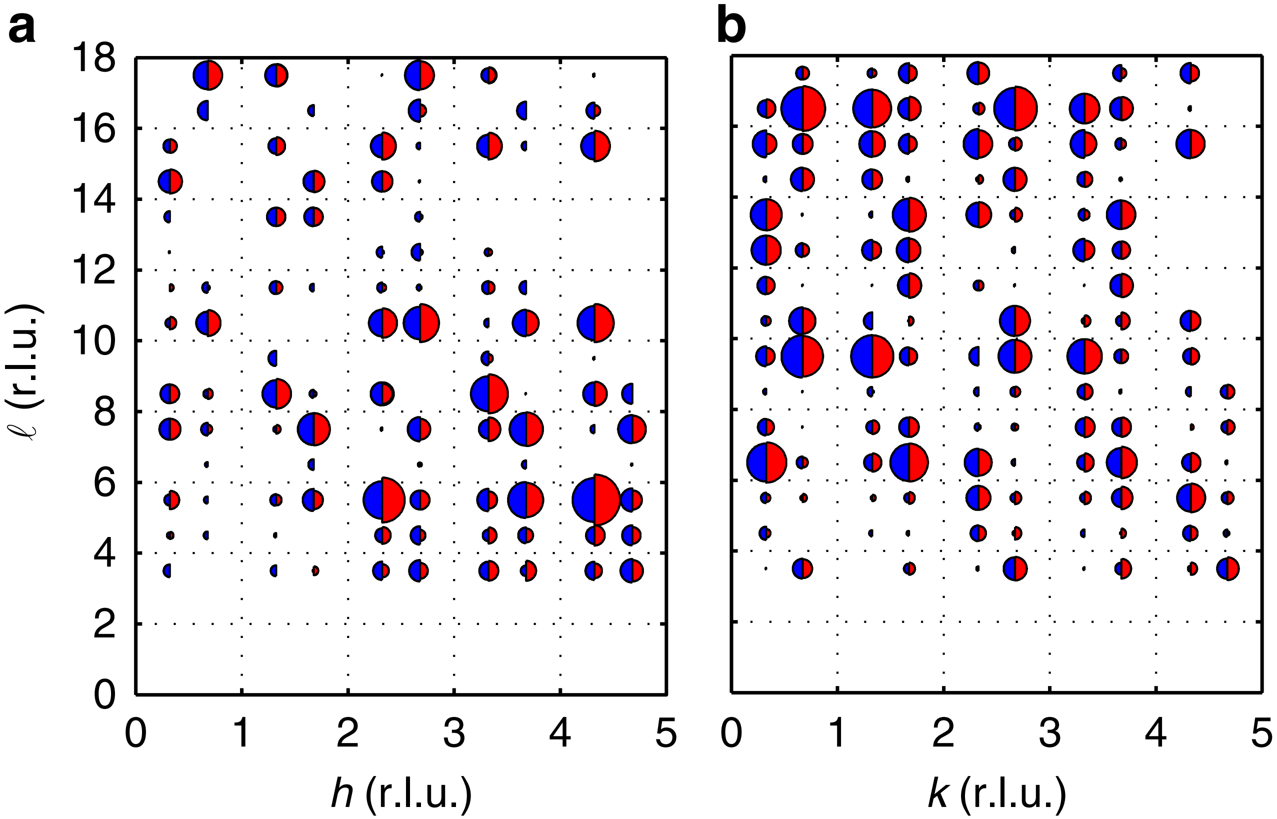


$$S = \sum_{j} f_j(Q)\exp(i\boldsymbol{Q}\cdot\boldsymbol{r}_j)$$

Out-of-plane distortions

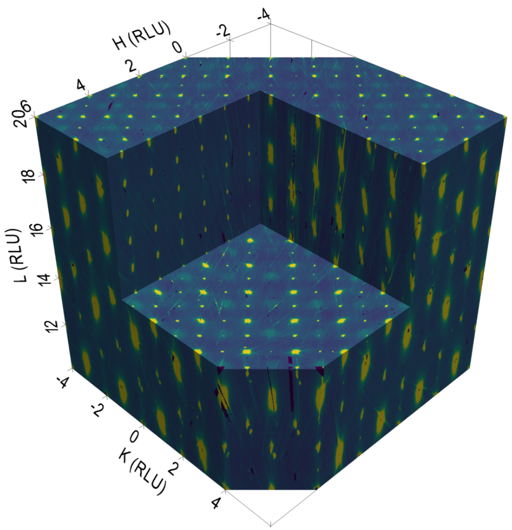
$YBa_2Cu_3O_{7-x}$

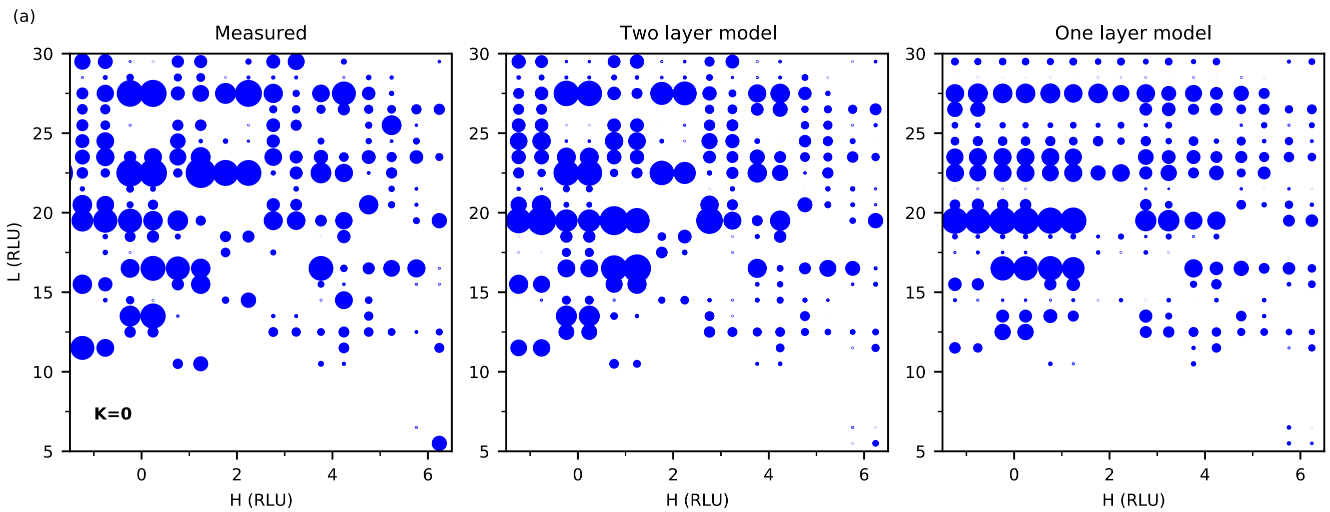


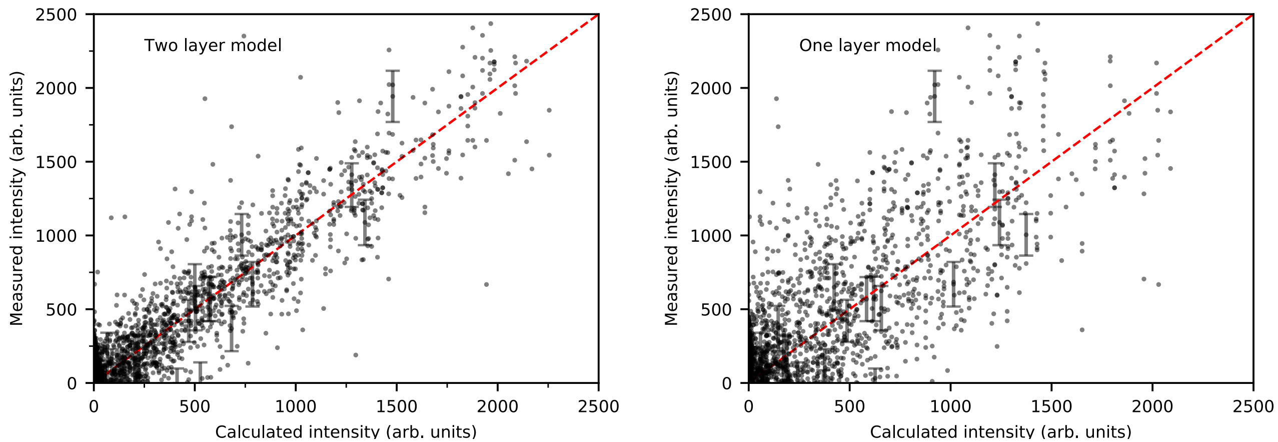


Nature Communications 6, *10064 (2015)*

3D – scattering volume







https://arxiv.org/pdf/2212.11964.pdf

Out-of-plane distortions

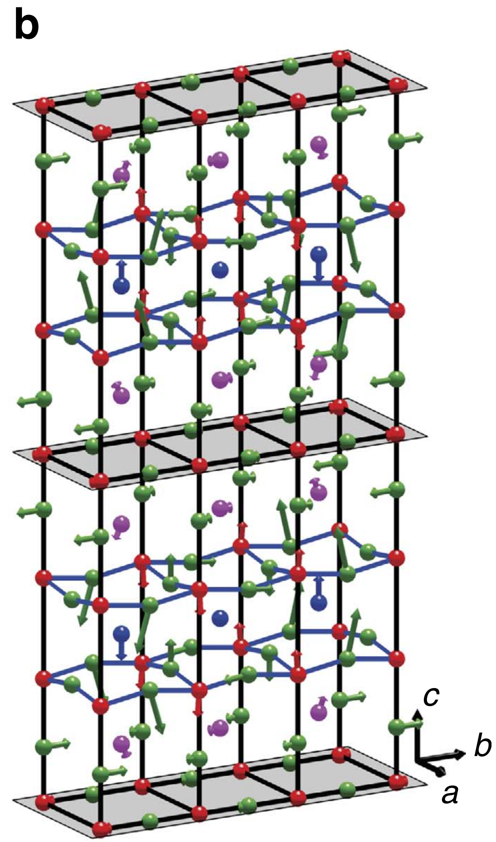
$YBa_2Cu_3O_{7-x}$

Table 1 | The values of fitted ionic displacements.

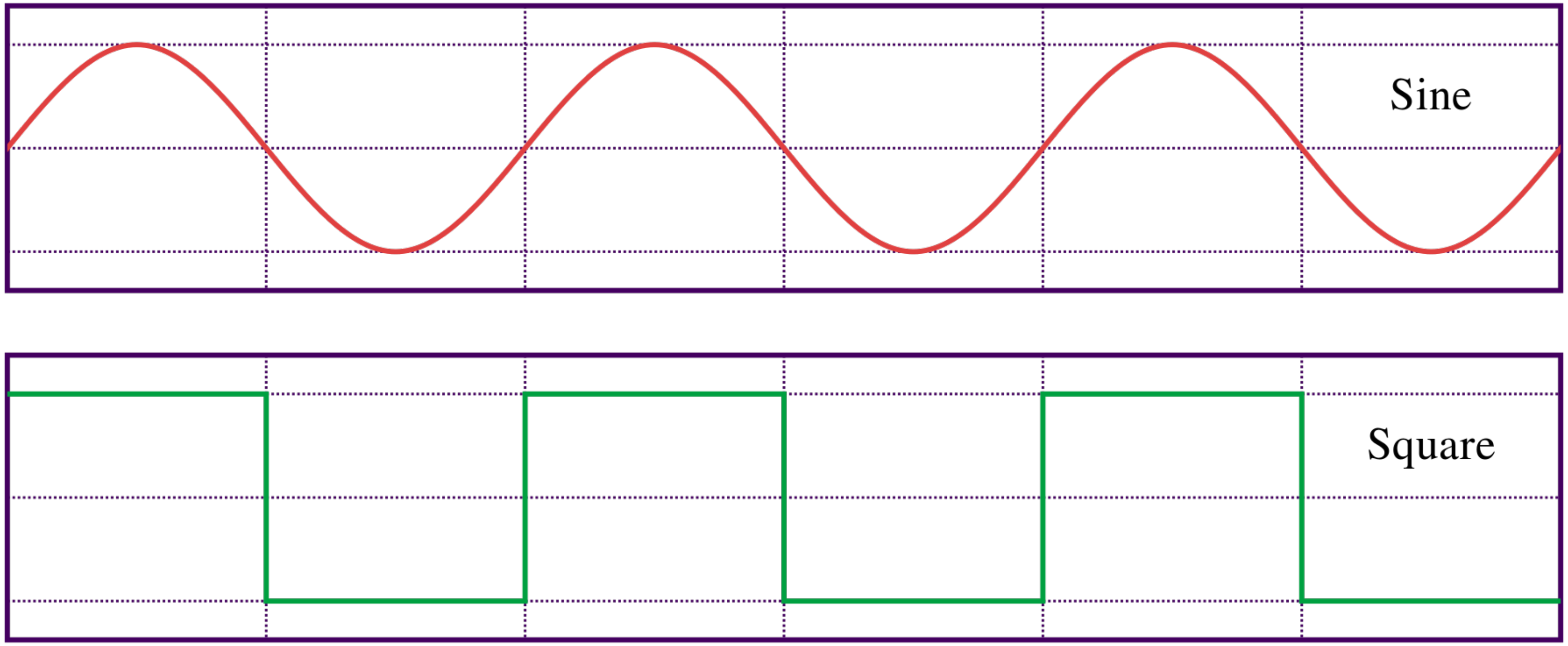
	u_c for $\mathbf{q}_b$	u_b for $\mathbf{q}_b$	u_c for $\mathbf{q}_b$	u_b for $\mathbf{q}_b$	$f(Q=0) \times u_c$ ($\mathbf{q}_b$)	$f(Q=0) \times u_b$ ($\mathbf{q}_b$)	u_c for $\mathbf{q}_a$	u_a for $\mathbf{q}_a$	$f(Q=0) \times u_c$ ($\mathbf{q}_a$)	$f(Q=0) \times u_a$ ($\mathbf{q}_a$)
Y	1.50 (3)	0	1.50 (3)	0	54 (1)	0	0.94 (6)	0	34 (2)	0
Ba	0.83 (2)	0.66 (3)	0.83 (2)	0.65 (2)	45 (1)	35 (1)	− 0.20 (2)	1.30 (5)	− 11 (1)	70 (3)
Cu (plane)	1.49 (3)	0.17 (5)	1.48 (3)	0.18 (5)	40 (1)	5 (1)	1.06 (5)	0.42 (6)	29 (2)	11 (2)
O_x (plane)	− 1.68 (16)	0.15 (30)	− 1.66 (15)	0.0 (0)	− 17 (2)	0 (0)	3.83 (30)	2.30 (42)	38 (3)	23 (4)
O_y (plane)	2.65 (16)	1.34 (30)	2.64 (16)	1.38 (27)	27 (2)	14 (3)	− 0.94 (28)	0.67 (40)	− 9 (3)	7 (4)
O (apical)	− 0.08 (18)	1.46 (24)	0.0 (0)	1.44 (23)	0 (0)	51 (9)	0.0 (0)	0.0 (0)	0 (0)	0 (0)
Cu (chain)	0	0.58 (7)	0	0.58 (7)	0	16 (2)	0	0.71 (9)	0	19 (3)
O (chain)	0	1.4 (2.7)	0	0.58 (0)	0	3 (0)	0	0.71 (0)	0	4 (0)
D-W α	4.9 (5)	4.9 (5)	4.8 (5)	4.8 (5)			6.2 (9)	6.2 (9)		
D-W β	3.3 (10)	3.3 (10)	3.2 (9)	3.2 (9)			4.8 (16)	4.8 (16)		
χ^2	1.01	1.01	1.00	1.00			0.96	0.96		

These are in absolute units, 10^{-3} Å, calculated, as described in Supplementary Note 4 and 5, from the fit of the data for the $\mathbf{q}_b$ and $\mathbf{q}_a$ modulated CDWs in ortho-II YBCO and subject to an overall possible systematic error ~50%, not included above. In the first two columns all variables are free, and in the second pair some values have been fixed and are marked by an error 0 in parentheses. Also given are the values multiplied by the scattering amplitude for each ion at $Q=0$ (the number of electrons on the ion) to emphasize the relative contributions of each ion to the amplitude. The *c*-components of the displacements are even about the yttrium layer of the crystal unit cell, and the horizontal displacements are odd. Displacements that are zero by symmetry are represented by 0. Below the displacements are given the fitted anisotropic Debye–Waller factors α and β, which appear in the expression: $\exp(-\alpha(Q_x^2+Q_y^2)-\beta Q_z^2)$. This multiplies the calculated intensities, and slightly improves the fit to the data, although the fitted displacements are little altered by including it. The units of α and β are 10^{-3} Å^2. The bottom row of the Table gives χ^2 per degree of freedom for the fits.

Nature Communications **6**, *10064 (2015)*

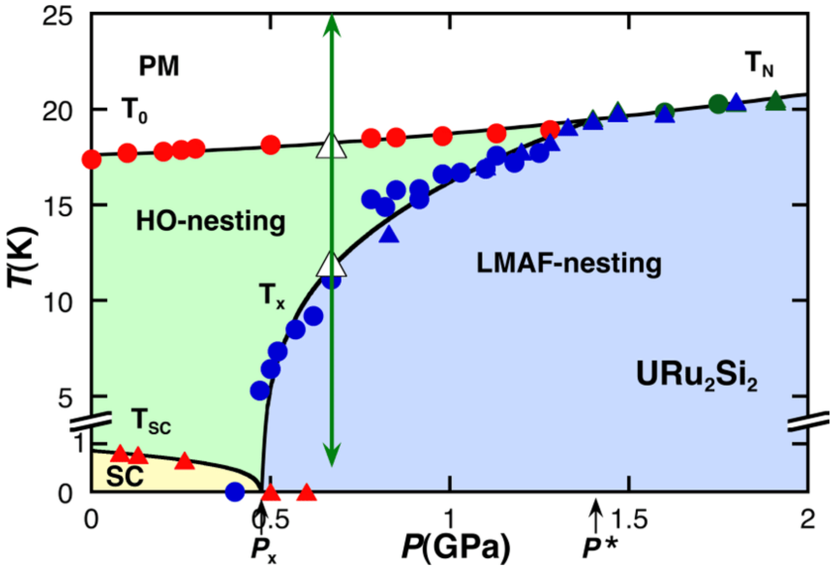


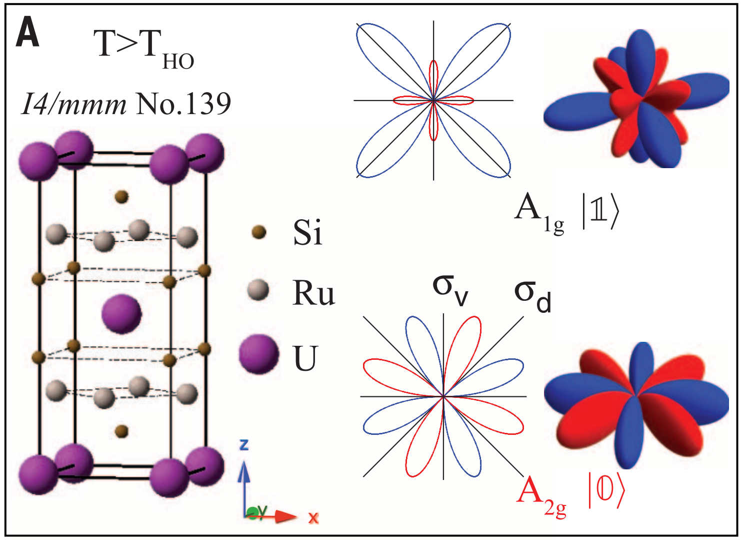
Difference between charge order and charge density wave

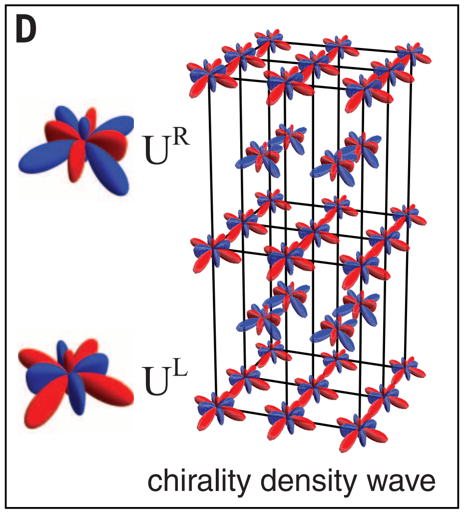


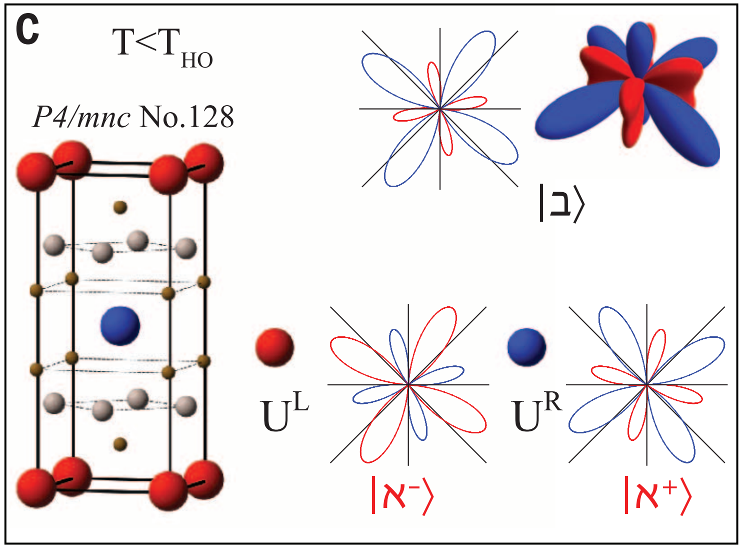
https://onlinetonegenerator.com

Hidden order problem: URu_2Si_2









Science 347, 1339 (2015)

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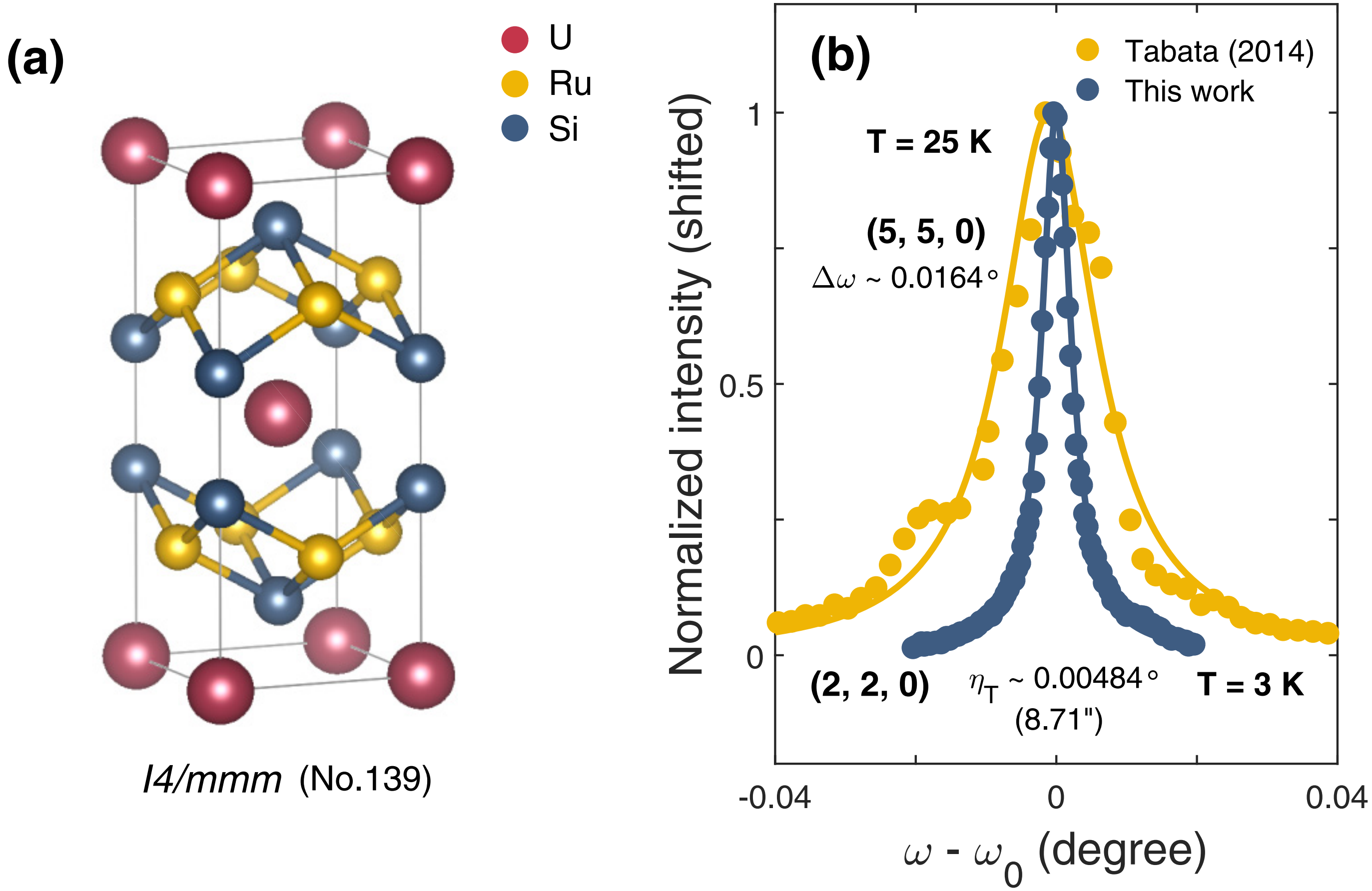
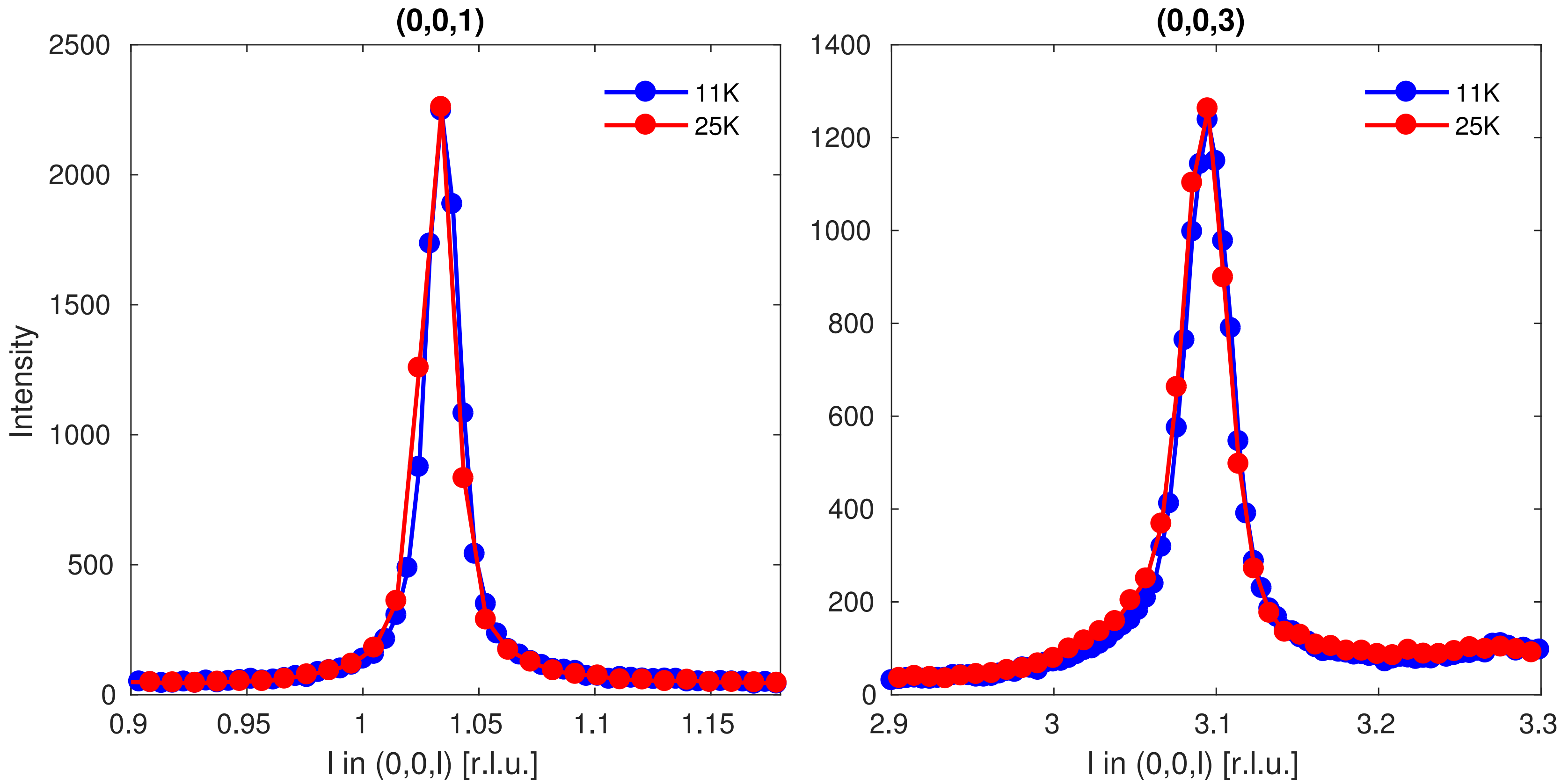
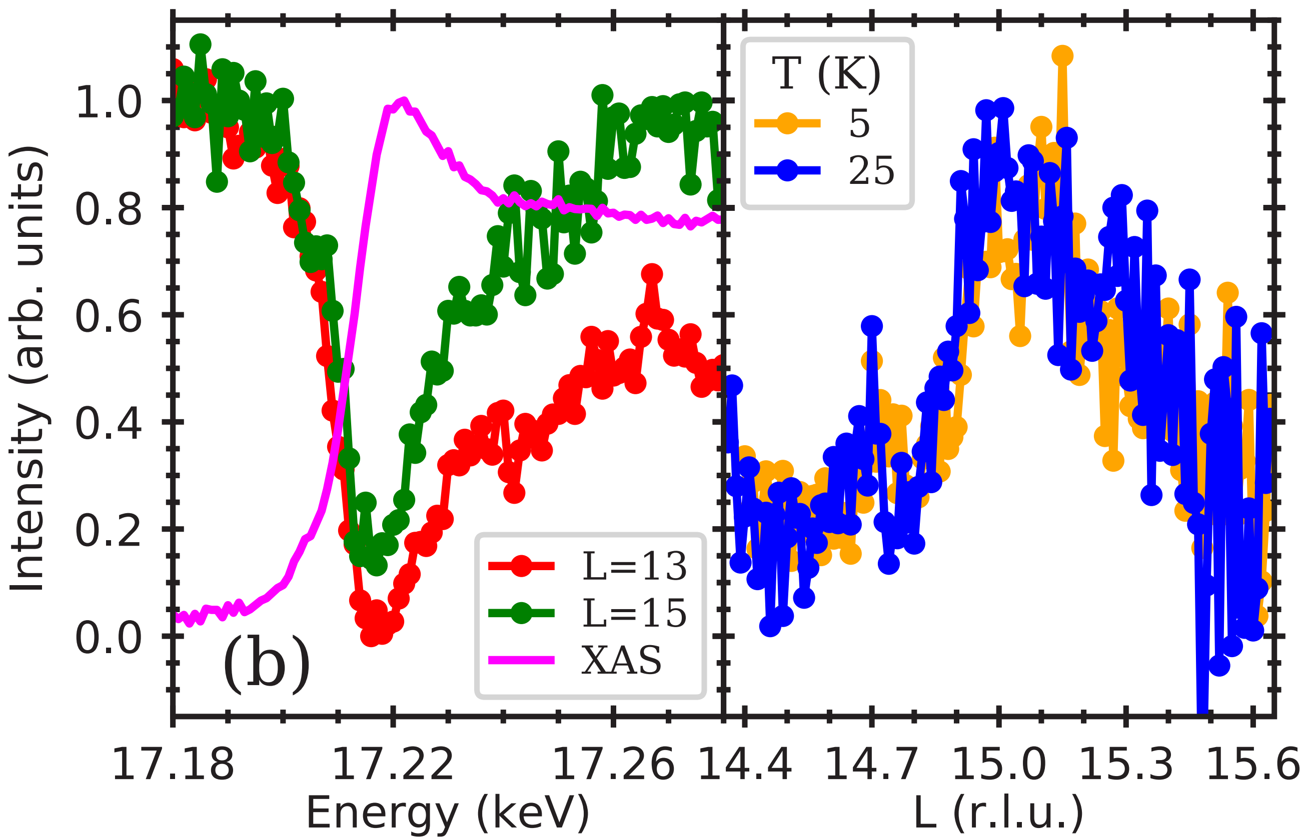

(a)
U
Ru
Si
I4/mmm (No.139)
(b)
Tabata (2014)
This work
T = 25 K
(5, 5, 0)
Δω ~ 0.0164°
(2, 2, 0)
η_T ~ 0.00484°
(8.71")
T = 3 K
Normalized intensity (shifted)
1
0.5
0
-0.04
0
0.04
ω - ω_0 (degree)

Hidden order problem: URu_2Si_2



Nik Dennler – Bachelor Thesis 2017

Hidden order problem: URu_2Si_2



PHYSICAL REVIEW B **96**, 085146 (2017)