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(United Kingdom)
john.helliwell@manchester.ac.uk
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<i>The Pore Wall Structure of Porous Semi-crystalline Anatase TiO₂</i>					
HE5525	J lwase, Kenji	Research Papers	Received by Co-editor (12 Feb 2011)	details	review document
<i>In situ lattice strain mapping by neutron transmission method and diffraction during tensile testing</i>					

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Journal Status		Papers this month	Keywords
JAC	Inactive until 2011-09-10	0	biological crystallography; synchrotron radiation instrumentation, methods and applications; neutron methods and applications

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The screenshot shows the IUCr World Directory website. The user is logged in as John Helliwell. The page displays the following information:

- Name:** John Richard Helliwell
- Current position:** Professor of Structural Chemistry
- Institution type:** University of Manchester
- Highest degree:** DSc awarded by U. York (1996) in Protein crystallography and molecular biophysics, Physics
- Address(es):** School of Chemistry, The University of Manchester, Brunswick Street, Manchester, M13 9PL, United Kingdom (map) (Professor of Structural Chemistry)
- Telephone number(s):** 44-161-275-4970 (Office)
- URL(s):** <http://www.manchester.ac.uk/research/John.helliwell/personaldetails>
- IUCr role(s):** Representative, ICSTI; Co-editor, Journal of Applied Crystallography; Member, IUCr/Oxford University Press (OUP) Book Series Selection Committee
- Scientific research interests:** anomalous dispersion, data collection and processing, enzymes, instrumentation, Laue diffraction, macromolecular crystallography, neutron scattering, powder diffraction, structural biology, structural chemistry, synchrotron radiation, teaching and education, time-resolved studies, X-ray optics.

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4.1. Log-in Information

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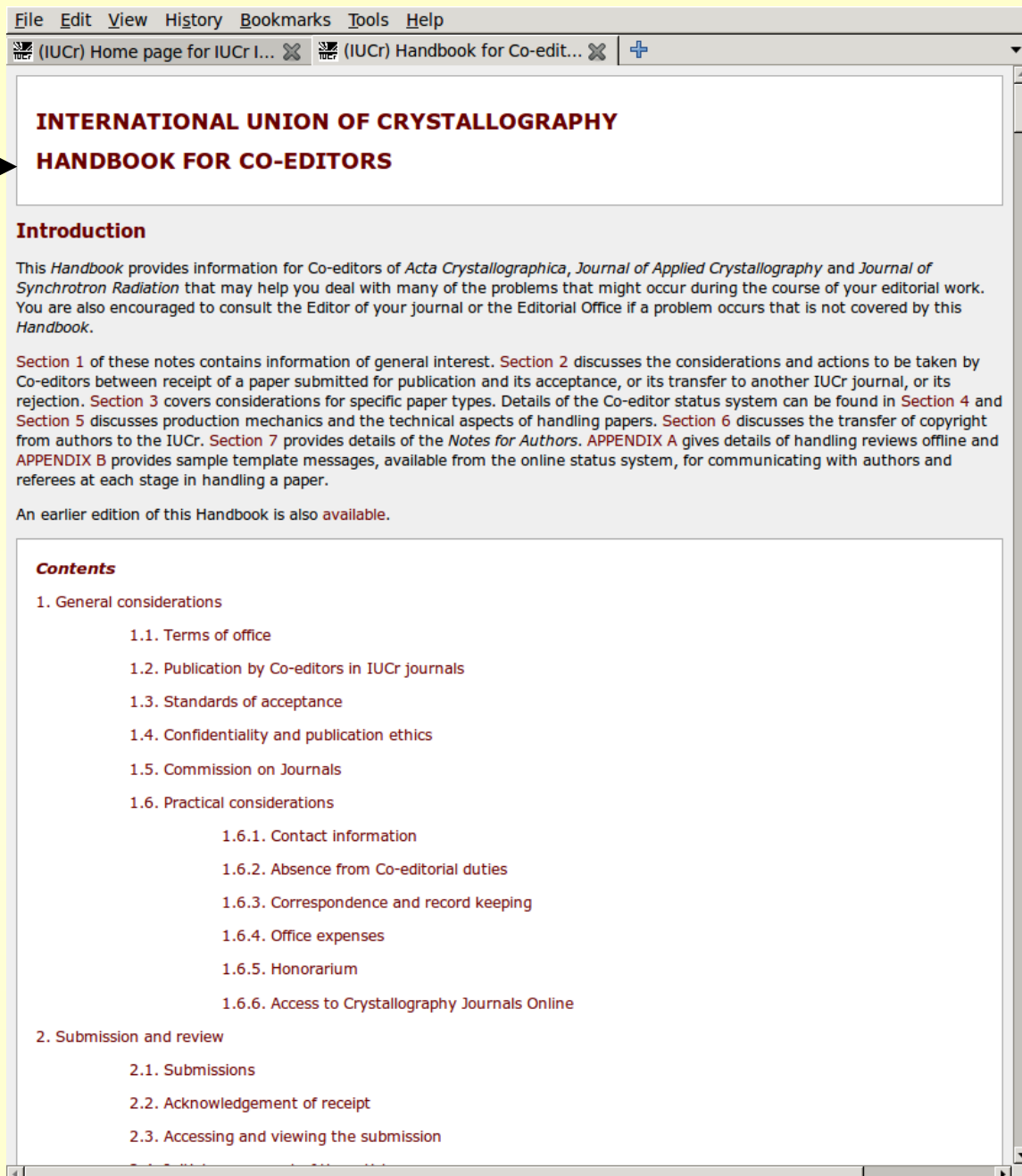
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4.2. Home page

Each Co-editor has a home page which contains the information described below. Co-editors receive details of the papers they are handling, showing the stage that each has reached in the publication process. The Main and Section Editors of journals receive the details of all Co-editors' papers. Details of any paper are always available from the Managing Editor.

- (1) **Personal details** - these are your details in the World Directory of Crystallographers. They can be edited by following the links **View/edit personal details** or **Edit e-mail details**. Making changes here will update your entry in the World Directory, but currently will not change your details in the submission system. If your details need to be updated in the submission system, contact support@iucr.org.
- (2) **Useful links** - these are links to online resources for Co-editors.
- (3) **Decisions** - this is a facility to allow you to accept, withdraw or reject a paper, and also to send an e-mail to the author informing them of your decision.
- (4) **Paper details** - this form allows you to jump directly to the article status page for a particular paper.
- (5) **Papers under review** - this table provides information about the papers you are handling. Papers that have been delayed are marked in red. In the list you will see a number of links. The **review document** button takes you to the EDITOR web page for an article and the **details** button takes you to the article status page (see [below](#)).
- (6) **Co-editor information** - this provides a summary of the information about the papers you are handling or have handled in the year. The information that is available is as follows:
 - (a) Papers received in the year.
 - (b) Delayed papers - a list of any papers that you are handling that have been under review for more than 6 months. The list can be sorted by Co-editor Code, Journal, Author, Category and Status. Each **details** button links to the article status page (see [below](#)).
 - (c) Papers under review - this is the same list as above.
 - (d) Papers not yet published - a list of all your papers that are currently under review or in the press.
 - (e) Full status list - all the papers that have been handled in the last year.
 - (f) New papers this month.
 - (g) Co-editor statistics - "number of papers received", "time to reach a decision" and "withdrawal and rejection rate", plus plots against the journal average for the last year and since records began. This page is updated monthly.
- (7) **Summary box** - this provides the number of submissions assigned to you as a Co-editor this month, plus whether you are "active" (i.e. some Co-editors ask not to be assigned papers if away on an extended trip), and the keywords that will appear in the

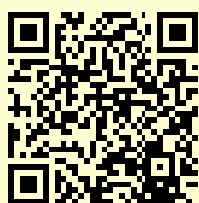
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AA	Albov, Dr Dmitry	Laboratory of Structural Chemistry Moscow State University Department of Chemistry Leninskiye Gory Moscow 119992	dmitryalbov@yandex.ru	E
AJ	Allen, Dr Andrew	National Institute of Standards and Technology 100 Bureau Drive Gaithersburg MD 20899-8523 USA	andrew.allen@nist.gov	J
AU	Authier, Professor Andre	Universite Pierre et Marie Curie, Villechenine, F-87470 Peyrat-le-Chateau, France	aauthier@wanadoo.fr	A
BQ	Büyükgüngör, Professor Dr Orhan	Ondokuz Mayıs University Department of Physics TR-55139 Samsun Turkey	orhanb@omu.edu.tr	E
BG	Baggio, Dr Ricardo	Departamento de Física, Comisión Nacional de Energía Atómica, CNEA, Av. Gral Paz 1499, 1650 Buenos Aires, Argentina	baggio@cnea.gov.ar	C,E
BE	Baker, Professor Ted	School of Biological Sciences, University of Auckland, Private Bag 92-019, Auckland, New Zealand	ted.baker@auckland.ac.nz	D
BA	Ballard, Dr Charles	CCP4, Daresbury Laboratory, Warrington, Cheshire WA4 4AD, England	charles.ballard@stfc.ac.uk	D
ZJ	Banerjee, Dr Rahul	Physical and Materials Chemistry Division National Chemical Laboratory Pune 411 008	r.banerjee@ncl.res.in	E
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UB	Beamer, Professor Lesa	117 Schweitzer Hall Department Biochemistry University of Missouri Columbia MO 65211 USA	beamerl@missouri.edu	F
BO	Bergfors, Terese	Department of Cell and Molecular Biology Biomedical Center Box 596 Uppsala University S-751 24 Uppsala Sweden	terese@xray.bmc.uu.se	F
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BH	Bernes, Professor Sylvain	DEP, Facultad de Ciencias Químicas, UANL Guerrero y Progreso S/N Col. Trevino 64570 Monterrey N.L. Mexico	sylvain_bernes@hotmail.com	E
ZB	Billing, Dr Dave	School of Chemistry University of the Witwatersrand Private Bag 3 PO Wits Johannesburg 2050 South Africa	dave.billing@wits.ac.za	B,E
IB	Billinge, Professor Simon	Department of Applied Physics and Applied Mathematics Columbia University 200 Mudd 500 W 120th Street New York NY 10027 USA	sb2896@columbia.edu	A
ZK	Biradha, Professor Kumar	Department of Chemistry Indian Institute of Technology Kharagpur 721 302	kbiradha@chem.iitkgp.ernet.in	E
ZQ	Blacque, Dr Olivier	Department of Inorganic Chemistry (ACI), University of Zürich, Winterthurerstrasse 190, 8057 Zürich, Switzerland	oblacque@aci.uzh.ch	E
BM	Blake, Professor Sandy	School of Chemistry, The University of Nottingham, University Park, Nottingham NG7 2RD, England	a.j.blake@nottingham.ac.uk	C
EB	Boldyreva, Professor Elena	Institute of Solid State Chemistry Russian Academy of Sciences ul. Kutateladze 18 Novosibirsk 128 Russia and Novosibirsk State University ul. Pirogova 2 Novosibirsk 90 Russia	eboldyreva@yahoo.com	B
BP	Bolotina, Dr Nadezhda	Institute of Crystallography Russian Academy of Sciences Leninsky prosp. 59 Moscow 119333 Russia	bolotina@ns.crys.ras.ru	B
BT	Bolte, Dr Michael	Institut für Anorganische Chemie, Goethe-Universität Frankfurt, Max-von-Laue-Str.7 D-60438 Frankfurt/Main, Germany	bolte@chemie.uni-frankfurt.de	E
BI	Bond, Dr Andrew	University of Southern Denmark Department of Chemistry Campusvej 55 5230 Odense M Denmark	adb@chem.sdu.dk	C,E

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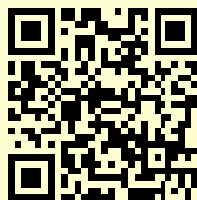
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AU	Authier, Professor Andre	Universite Pierre et Marie Curie, Villechenine, F-87470 Peyrat-le-Chateau, France	aauthier@wanadoo.fr	A
IB	Billinge, Professor Simon	Department of Applied Physics and Applied Mathematics Columbia University 200 Mudd 500 W 120th Street New York NY 10027 USA	sb2896@columbia.edu	A
CC	Carter, Professor Charlie	Department of Biochemistry University of North Carolina School of Medicine Chapel Hill NC 27599 7260 USA	carter@med.unc.edu	A
DM	Dmitrienko, Professor Vladimir	Institute of Crystallography Leninsky pr.59 Moscow 117333 Russia	dmitrien@ns.crys.ras.ru	A
EO	Eon, Professor Dr Jean-Guillaume	Instituto de Quimica Universidade Federal do Rio de Janeiro Cidade Universitaria - Ilha do Fundao Rio de Janeiro 21945-970, Brazil	jgeon@iq.ufrj.br	A
KX	Kuhs, Professor Dr Werner	Georg-August University Gottingen GZG Crystallography Goldschmidtstr. 1 D-37077 Gottingen Germany	wkuhs1@gwdg.de	A
MQ	Miao, Professor John	Department of Physics and Astronomy University of California Box 951547 Los Angeles CA 90095-1547 USA	miao@physics.ucla.edu	A
MK	Millane, Professor Rick	Department of Electrical and Computer Engineering University of Canterbury Private Bag 4800 Christchurch New Zealand	rick.millane@canterbury.ac.nz	A
PC	Petricek, Dr Vaclav	Department of Structures Analysis Institute of Physics Academy of Sciences of the Czech Republic, v.v.i. Cukrovamicka 10 162 00 Praha 6 Czech Republic	petricek@fzu.cz	A
SC	Schenk, Professor Henk	Laboratorium voor Kristallografie HIMS, FWNI, University of Amsterdam Valckenierstraat 65 1018XE Amsterdam The Netherlands	h.schenk@uva.nl	A
SH	Schwarzenbach, Professor Dieter	Ecole Polytechnique Fédérale Laboratory of Crystallography EPFL-FSB-IPMC-LCr Le Cubotron CH-1015 Lausanne Switzerland	dieter.schwarzenbach@epfl.ch	A
WX	Steurer, Professor Walter	Laboratory of Crystallography Wolfgang-Pauli-Strasse 10 ETH Zurich CH-8093 Zurich Switzerland	steurer@mat.ethz.ch	A
TN	Tanaka, Professor Kiyo	Department of Materials Science and Engineering, Nagoya Institute of Technology, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan	tanaka.kiyoaki@nitech.ac.jp	A
TD	Tsuda, Professor Kenji	Institute of Multidisciplinary Research for Advanced Materials Tohoku University 2-1-1 Katahira Aoba-ku Sendai 980-8577 Japan	k_tsuda@tagen.tohoku.ac.jp	A
WL	Wilkins, Professor Steve	CSIRO, Materials Science and Engineering, Private Bag 33, Clayton South MDC, VIC 3169, Australia	steve.wilkins@csiro.au	A
WO	Willmott, Professor Philip	Swiss Light Source Paul Scherrer Institute CH-5232 Villigen Switzerland	philip.willmott@psi.ch	A
ZM	Zimmermann, Professor Helmut	Institut für Physik der kondensierten Materie Universität Erlangen Staudtstrasse 3 D-91058 Erlangen Germany	zimmermann@kristuni-erlangen.de	A
PZ	Perez-Mato, Professor Manu	Dept Fisica de la Materia Condensada Universidad del Pais Vasco Apdo 644 48080 Bilbao Spain	wmppemam@lg.ehu.es	A,B
PF	Paufler, Professor Peter	Institut für Strukturphysik, Fachrichtung Physik, Fakultät Mathematik und Naturwissenschaften, Technische Universität Dresden, D-01062 Dresden Germany	paufler@physik.tu-dresden.de	A,B,C,D,E,F,J,S
ME	Strickland, Peter	5 Abbey Square, Chester CH1 2HU, UK	med@iucr.org	A,B,C,D,E,F,J,S
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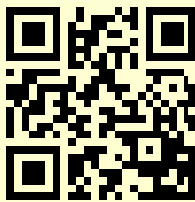
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<i>Acta B</i>	10	6	5	25	0	0	8	0	details
<i>Acta C</i>	49	28	24	49	1	-6	12	27	details
<i>Acta D</i>	18	13	0	38	0	0	10	8	details
<i>Acta E</i>	478	391	93	252	1	-1	72	407	details
<i>Acta F</i>	33	27	2	71	0	0	17	25	details
<i>JAC</i>	18	19	10	67	1	1	30	0	details
<i>JSR</i>	20	11	6	55	0	0	10	3	details
Total	635	497	150	585	3	-7	166	475	

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JComm 2011 meeting

August 19-21, Euroforum Infantes, San Lorenzo de El Escorial, Spain

Meeting details



Agenda

Draft agenda papers are now available. It is intended that the agenda will allow for discussions, demonstrations and talks on best practice.

Approximate timetable of events

19th - Arrival in afternoon; short opening evening session
20th - 09:00-17:00 - Individual journal sessions
21st - 09:00-11:00 - Individual journal sessions
21st - 11:00-13:00 - Plenary session
Close of meeting

Registration

To register for the meeting, click [here](#). The IUCr will pay for meals and accommodation for the duration of the meeting. Grants towards travel costs may be available (see the registration form).

Details of the venue

Euroforum Infantes
C/ del Rey, 38
San Lorenzo de El Escorial
28200 Madrid
Spain

Web site: <http://www.euroforum.es/index.php?q=en>

Telephone: +34 91 896 70 00
Fax: +34 91 896 70 70
E-mail: info@euroforum.es

Wifi is available at the venue. Meeting rooms and bedrooms are all air conditioned. Smoking is not permitted in the venue.

How to reach Euroforum Infantes

By car: From Madrid, take the A6, exit at milestone 47 to San Lorenzo de El Escorial (M-600 road). Alternatively, take the A6, exit

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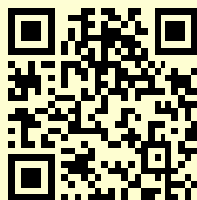
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Helliwell, Professor
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HE5525	J lwase, Kenji	Research Papers	Received by Co-editor (12 Feb 2011)	details	review document
<i>In situ lattice strain mapping by neutron transmission method and diffraction during tensile testing</i>					

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JAC	Inactive until 2011-09-10	0	biological crystallography; synchrotron radiation instrumentation, methods and applications; neutron methods and applications

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HE5512	Bull, Craig	craig.bull@stfc.ac.uk	Research Papers	Published (13 Jul 2011) details
<i>High-Pressure Single-Crystal Neutron Diffraction to 10 GPa by Angle-Dispersive Techniques</i>				
HE5510	Lynch, Peter Adrian	Peter.Lynch@csiro.au	Research Papers	Published (14 May 2011) details
<i>A uni-axial tensile stage with tracking capabilities for micro X-ray diffraction applications</i>				

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<i>The Pore Wall Structure of Porous Semi-crystalline Anatase TiO2</i>				
HE5525	Iwase, Kenji	fbwase@mx.ibaraki.ac.jp	Research Papers Received by Co-editor (12 Feb 2011)	details review document
<i>In situ lattice strain mapping by neutron transmission method and diffraction during tensile testing</i>				

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<i>In situ lattice strain mapping by neutron transmission method and diffraction during tensile testing</i>				
HE5512	Bull, Craig	craig.bull@stfc.ac.uk	Research Papers	Published (13 Jul 2011) details
<i>High-Pressure Single-Crystal Neutron Diffraction to 10 GPa by Angle-Dispersive Techniques</i>				
HE5529	Wood, Peter A.	wood@ccdc.cam.ac.uk	Computer Programs	Published (8 Jun 2011) details
<i>New Software for Statistical Analysis of CSD Data</i>				
HE5530	Macchi, Piero	piero.macchi@dcb.unibe.ch	Research Papers	Published (8 Jun 2011) details
<i>Low energy contamination of Mo micro-source X-ray radiation: analysis of the problem and solution</i>				
HE5523	Tanaka, Isao	tanaka@castor.sci.hokudai.ac.jp	Research Papers	Published (8 Jun 2011) details
<i>In-crystal affinity ranking of fragment hit-compounds revealed a relationship with their inhibitory activities.</i>				
HE5524	Schreiber, Frank	thilo.stehle@uni-tuebingen.de	Research Papers	Published (8 Jun 2011) details
<i>Novel Approach to Controlled Protein Crystallization through Ligandation of Yttrium Cations</i>				

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Jul 2010 – Jun 2011												
Total number of papers received	Number of papers received	Time to reach a decision (months)	Combined withdrawal and rejection rate (%)	Allocated this month	Number in review	The combined withdrawal and rejection rate is based on the total number of articles accepted, rejected and withdrawn in the previous 12-months.						
Journal	You	Journal	You	Journal	You	Journal	You	Journal	You	Journal	You	
JAC	283	4272	32	242	3.50	3.73	33.33	33.20	0	17	2	69

average decision time

JAC

— Journal decision time. — Co-editor decision time. — Number of papers Co-editor average based on

The average decision time is based on the number of papers that reached a status of accepted, withdrawn or rejected in the previous 12-months.

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<i>In situ lattice strain mapping by neutron transmission method and diffraction during tensile testing</i>					

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Journal Status	Papers this month	Keywords
JAC Inactive until 2011-09-10	0	biological crystallography; synchrotron radiation instrumentation, methods and applications; neutron methods and applications



Journal	Status	Papers this month	Keywords
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Man-Ho Kim*, Jeong-Mann Doh, Seong Chul Han, Keun Hwa Chae, Byung-Yong Yu, Kyung Tae Hong, Andrew Jackson and Lawrence Anovitz

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<i>In situ lattice strain mapping by neutron transmission method and diffraction during tensile testing</i>					

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The Pore Wall Structure of Porous Semi-crystalline Anatase TiO2

Man-Ho Kim*, Jeong-Mann Doh, Seong Chul Han, Keun Hwa Chae, Byung-Yong Yu, Kyung Tae Hong, Andrew Jackson and Lawrence Anovitz (man-hokim@kist.kr)

Co-editor: **Professor J.R. Helliwell Strickland** Paper type: **research papers** IUCr contact: **Peter**

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- suggest an alternative journal

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- thank reviewer
- ask reviewer to check revised article
- inform reviewer of decision

Request revision to paper


- pre-review revision
- request a revision

Decisions

- accept paper for publication
- withdraw paper
- reject paper
- accept paper and transfer it to another journal

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man-hokim@kist.kr	ps@iucr.org	Receipt of your submission to Journal of Applied Crystallography	2011-04-07 09:09:22
man-hokim@kist.kr	ps@iucr.org	Article he5531: Co-editor assignment	2011-04-07 10:42:26
ps@iucr.org	online.submission.j@iucr.org	Article he5531: new submission he5531 to Journal of Applied Crystallography	2011-04-07 10:42:26
ajj@nist.gov,yu2997@kist.ac.kr	online.submission.j@iucr.org	Article submission (reference: he5531)	2011-04-07 10:42:26
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High-pressure single-crystal neutron diffraction to 10 GPa by angle-dispersive techniques

C.L. Bull, M. Guthrie, J. Archer, M.-T. Fernandez-Diaz, J.S. Loveday, K. Komatsu, H. Hamidov and R.J. Nelmes (craig.bull@stfc.ac.uk)

Co-editor: **Professor J.R. Hellwell**

Paper type: **research papers**

IUCr contact: **Peter Strickland**

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Article published online

	HTML	Fri Jul 22 13:32:06 2011
	PDF	Fri Jul 22 13:32:12 2011
	Review PDF	Wed May 25 16:44:43 2011
	Proof (PDF)	Thu Jun 16 10:38:29 2011

Review from referee 1 (John Evans)

Referee 1's report

Review report:

High pressure single crystal diffraction is an important area of modern crystallographic research and this team are world-leaders in the area. Over recent years they have made a number of important technique developments allowing the study of many important phenomena. I was therefore very interested to receive this paper on accessing pressures up to 10 GPa with constant wavelength neutrons, a significant increase over what has been possible.

Unfortunately I didn't find the paper definitely informative.

Section 5 on alignment says little more than "apparatus is assembled carefully so things are well aligned".

My major objection to the paper is that it is about measuring high precision data at high pressure. However the only real data really presented is on the use of collimation to increase signal to noise. There are no data sets at pressure presented, no refinements discussed to show good results can be obtained, no look at e.g. merging R-factors to assess data precision. I've no reason to doubt that they can record good data, but there is nothing presented in the paper. It's not even clear if the single intensity measurement presented (Fig 4) was recorded at pressure.

I also found section 9 of the paper rather strange. The first 1/3 seems to highlight work that's already been published. The next section is on experiments underway but with no concrete results as yet. The final portion is about what the authors would like to help with sample preparation.

Overall I'm afraid that I don't support publication of the paper. There is insufficient crystallography present and no data presented to show that useful high precision data can be obtained at high pressure.

Is the paper worthy of publication?	no, not at all
What do you think the impact of the article will be (1=low, 5=high)?	2
Is the choice of journal correct?	yes
Is the work technically sound?	yes
Does the evidence presented justify the conclusions drawn?	no
Could the presentation be more efficient?	yes
Can any material be omitted or deposited?	yes
Should any additional graphics/multimedia be included?	no
Have the requirements of the Notes for Authors been met?	yes
Is the literature adequately cited?	yes

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Man-Ho Kim*, Jeong-Mann Doh, Seong
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man-hokim@kist.kr	ps@iucr.org	Receipt of your submission to Journal of Applied Crystall	2011-04-07 09:09:22
man-hokim@kist.kr	ps@iucr.org	Article he5531: Co-editor assignment	2011-04-07 10:42:26
ps@iucr.org	online.submission.j@iucr.o	Article he5531: new submission he5531 to Journal of Ap	2011-04-07 10:42:26
ajj@nist.gov,yu2997@kist.	online.submission.j@iucr.o	Article submission (reference: he5531)	2011-04-07 10:42:26
john.helliwell@manchester.	ps@iucr.org	Article he5531: new submission he5531 to Journal of Ap	2011-04-07 10:42:26
man-hokim@kist.kr	Professor J.R.Helliwell <on	Article he5531	2011-04-07 19:29:54
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Man-Ho Kim*, Jeong-Mann Doh, Seong Jackson and Lawrence Anovitz

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J. Appl. Cryst. (2010). 43, 1-7 [doi:10.1107/S00218898090044112]

In-situ small-angle neutron scattering study of pore filling and pore emptying in ordered mesoporous silica

M. Erko, D. Wallacher, A. Brandt and O. Paris

Abstract: The capillary condensation and capillary emptying of water and perfluoropentane in ordered mesoporous SBA-15 silica is studied by *in-situ* small-angle neutron scattering (SANS). The SANS data can be perfectly described by a simple analytical model for spatially random pore filling (Laue

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The Pore Wall Structure of Anatase TiO2

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Authors: Man-Ho Kim*, Jeong-Mann Doh, Seong Chul Han, Keun Hwa Chae, Byung-Yong Yu, Kyung Tae Hong, Andrew Jackson and Lawrence Anovitz
Title: The Pore Wall Structure of Porous Semi-crystalline Anatase TiO2

There are lots of errors of the first kind. The authors should carefully examine the manuscript before submission. These errors impose difficulties on this reviewer to read through the manuscript and to judge the work fairly.

- (1) Although, the authors presented the results of FESEM in Figure 1, there is no description on the FESEM in the section of Experimental Methods.
- (2) Page 3 location 021; "Second level heading (style: IUCr heading 2)" should be dropped out.
- (3) Page 5 location 057; Figure 3-(a) is perhaps Figure 5-(a)?
- (4) Page 9 location 010; Figure 4 is perhaps Figure 6?
- (5) Page 9 location 040; What is "fom"?
- (6) Page 10 location 016; Figure 4 is perhaps Figure 6?
- (7) Page 10 location 019; Figure 4-(a) is perhaps Figure 6-(a)?
- (8) Page 10 location 024; Figure 4-(b) is perhaps Figure 6-(b)?
- (9) Following descriptions are also editing errors.
- (10) Page 5 location 023; "FESEM(superscript18)"
- (11) Page 5 location 047; "the beam direction (ref.18)"
- (12) Page 6 location 016; There is no "part.B" in this manuscript. What is "part.B"?

Major concern:

The authors have already obtained a fairly good morphological image of the porous structure by FESEM measurement as shown in Figure 1. In reality they utilized some structural parameters that were obtained by FESEM, when they analyzed the scattering curve of neutron scattering. Then, what is the merit of the neutron scattering? In other words, what cannot be done by FESEM? It is often claimed that the scattering method can observe the averaged structure. However, the averaging is also possible by the microscopic technique if wider area is scanned. Probably, detailed information that is embedded within the apparent morphology will be a good instance. Therefore, the authors applied a contrast matching method to obtain the mass density of the porous structure. So the last part of the manuscript is considered to be the core of the present work. The authors showed a contrast-matching plot only for a certain scattering vector. This is not enough. They should show a flat scattering curve to validate the contrast-matching condition.

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Man-Ho Kim*, Jeon Anovitz (man-hokim@kist.kr)

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due to the presence of fluorine and carbon partially absorbed by the pore wall from the fluoride-containing electrolyte and sorbed water molecules on the wall. The neutron contrast-matching point between the TiO₂ matrix and the pores filled with liquid H₂O/D₂O mixtures was 51/49 vol/vol H₂O/D₂O, yielding an estimated mass density of 3.32 g/cm³. The specific surface area of the sample derived from the (U)SANS data, S/V, was around 939 ~ 1003 m²/cm³ (283~ 302m²/g).

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Analytical Description of the Scattering of Cellulose Nanocrystals in Tracheid Wood Cells

Peter Strickland*

Abstract

Tracheid cells are complex structures. The cellulose nanocrystals are wound in helices around the tracheid cell axis. The microfibril angle (MFA) describes the angle between the cellulose crystals and the cell axis. Furthermore, the cross-sectional shape of tracheids varies widely, ranging from square to round. These parameters affect the scattering geometry and thus the experimental scattering signal. In an experiment, the macroscopic sample orientation relative to the beam is a further variable. Here, we present a description that allows for the calculation of azimuthal scattering patterns for any hkl reflection from cellulose nanocrystals in tracheid cells of any orientation. Additionally, this model can be used to describe fibrillar aggregates with an additional level of organization that surpasses an ideal fiber texture, for example pairs of twisted fibers.

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The present paper shows how the growing computational power of modern GPUs can be employed to simulate the diffraction pattern of nanostructured materials. Details on the implementation of the Debye equation in C for CUDA (Compute Unified Device Architecture) code and perspectives in this new field are presented with some examples of pattern simulations.

2. GPU

2.1. A brief history of Graphics Processing Units

The path towards GPU computing began with non-programmable graphics accelerators in the 1980s. Video boards were available, directly driven by the CPU but mounting on board all the logics necessary to provide text and buffered graphical output on a raster screen. By the mid-1990s it became possible to integrate the video controls as well as some logics onto a single chip (?), but only in 1999 the first true GPUs were presented with the specific aim of offloading 3D graphics rendering from the CPU (?).

Attracted by the impressive floating-point performances, some scientist began using GPUs for non-graphical applications: in 2002 Mark Harris (?) coined the term General-Purpose computation on Graphics Processing Units (GPGPU), effectively starting a new scientific computing era. In the early times, GPU computing was really difficult, as it was based on parasitic use of graphics Application Programming Interfaces (APIs). Programmers were forced to turn data into images/textures and algorithms into image/texture processing: an intimate knowledge of graphics APIs and GPU architecture was thus required.

Despite this intrinsic difficulty, the academic world quickly realized the potentiality of the GPUs, developing new high-level languages and programming environments for

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Peter Strickland*

Abstract

Tracheid cells are complex structures. The cellulose nanocrystals are wound in the microfibril angle (MFA) describes the angle between the cellulose crystals in cross-sectional shape of tracheids varies widely, ranging from square to round, scattering geometry and thus the experimental scattering signal. In an experiment orientation relative to the beam is a further variable. Here, we present a description of azimuthal scattering patterns for x-ray reflection from cellulose nanocryst organization. Additionally, this model can be used to describe fibrillar aggregates organization that surpasses a model fiber texture, for example pairs of twisted

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
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

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High-pressure single-crystal neutron diffraction to 10 GPa by angle-dispersive techniques

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has now been accepted for publication in Journal of Applied Crystallography.

Thank you again for your review of this article, which is much appreciated.

Best wishes

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man-hokim@kist.kr	Professor J.R.Helliwell <on	Article he5531	2011-04-07 19:29:54
man-hokim@kist.kr	ps@iucr.org	Article he5531: revised article submitted	2011-04-08 11:18:01



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papers under review

HE5531	J Kim, Man-Ho	Research Papers	Received by Co-editor (7 Apr 2011)	details	review document
<i>The Pore Wall Structure of Porous Semi-crystalline Anatase TiO2</i>					
HE5525	J lwase, Kenji	Research Papers	Received by Co-editor (12 Feb 2011)	details	review document
<i>In situ lattice strain mapping by neutron transmission method and diffraction during tensile testing</i>					

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our submission to Journal of Applied Crystallography	2011-04-07 09:09:22
31: Co-editor assignment	2011-04-07 10:42:26
31: new submission he5531 to Journal of Applied Crysta	2011-04-07 10:42:26
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2 11:33:12
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