European Structural Integrity Society

ESIS Newsletter #50, August, 2012

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EDITORIAL BY THE ESIS PRESIDENT

We are all looking forward to ECF 19 in Kazan which will take place from August 26 until August 31. It is expected that there will be over 400 participants. The conference will be held at the Korston Hotel and Mall.

I would like to share with you the progress that ESIS has made since the last newsletter. We have a new set of Statutes that was approved by the ESIS Council. With the new Statutes, we are seeking to be recognized as an official European Society. The ExCo has proposed registration in the UK through our Secretary James Marrow.

Our blog in which Wolfgang Brocks reviews different papers from Engineering Fracture Mechanics continues to receive attention. This information may be found through our web site at www.structuralintegrity.eu or from the direct link www.imechanica.org/blog/23810 . Wolfgang has reviewed four papers and over 9,000 people have looked at the reviews. There have been a number of interesting responses. I would like to encourage you to read these interesting pieces and respond.

All of the proceedings from previous ECF meetings (except for ECF 1) have been digitized and are available on the ESIS website for ESIS members. I want to thank Francesco Iacoviello for this excellent contribution to ESIS. I will also

remind you that ESIS members can access all ESIS documents through the website.

The Executive Committee at their meeting in Berlin in May, 2012, proposed canceling awards at ECF19. This difficult decision was submitted to the Council by e-mail and approved. More details are given in the Newsletter. In addition, it was decided to call for an e-mail vote by the ESIS Council for the revised ESIS Statutes before the Council meeting in Kazan. This was done for two reasons. First, there are many issues to discuss on the Council meeting agenda at Kazan including the choice of a venue for ECF 21. Second, with the revised Statutes, we have been able to proceed with registering ESIS as an official organization in Europe. Council members received the Statutes twice in order to suggest changes and make comments. The statutes were changed twice at their request and approved. Out of 30 possible votes, 28 people voted with 27 for the new Statutes and one abstention. The Executive Committee appreciates the excellent turn-out and support for the new Statutes.

Recall that we publish Special Issues in the three Elsevier journals which we support: Engineering Fracture Mechanics, International Journal of Fatigue, and Engineering Failure Analysis. The newest Special Issues include:

1. A. Carpinteri, L. Pook and A. Spagnoli (eds) Multiaxial Fracture (ICMFF9 Multiaxial Fatigue), Engineering Fracture Mechanics, Vol. 78, Issue 8 (2011).

2. E. Macha and D. Rozumek (eds.) Physical and Phenomenological Approaches to Fatigue Damage (TC3), International Journal of Fatigue, Vol. 39 (2012).

I want to thank the TC-Chairs that made this very important contribution to ESIS. We expect more issues this year and I would like to encourage other TC-Chairs to submit Special Issues related to their research.

I would like to encourage all of you to look at our website and join a TC (Technical Committee) which is close to your area of expertise. The TCs hold very interesting small and medium sized meetings. If you are interested in starting a new TC, please contact me and we will try to arrange it with the necessary approval.

In addition, we have been busy with other activities. Antonio Martin-Meizoso and Liviu Marsavina have prepared a presentation for TC-Chairs which will take place on Wednesday, August 29, at 3:00 at ECF 19 concerning application for funds from COST to support their activities. In addition, they are proposing the establishment of a Summer School to be held before ECF meetings. I look forward to your support for these new activities. I wish to thank Antonio and Liviu for their efforts.

Finally, I am pleased to announce the election of new ESIS fellows who will be awarded their certificates at the Banquet in Kazan. They include:

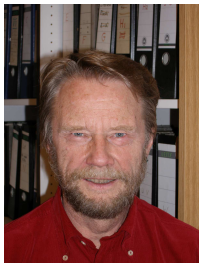
1. Andrea Carpinteri is a Professor of Structural Mechanics at the University of Parma. He is being awarded this honor for his outstanding research in theoretical and numerical modeling of materials and structures; fracture mechanics of engineering materials and structures; reinforced and fibre-reinforced concrete structures; and time-variable and seismic loadings; as well as, his seminal contribution to TC-3 as co-chair and to ESIS.
2. Otmar Kolednik is a Professor of Materials Science at the Austrian Academy of Sciences and the University of Loeben. He is being awarded this honor for his outstanding research in the relation between the micro- and nanostructure of materials and their deformation and fracture properties; the development of new testing procedures to measure local deformation and fracture properties; the theoretical concepts of non-linear fracture mechanics, and the numerical modeling of plastic deformation, damage initiation and crack growth under monotonic and cyclic loading. He has been a member of TC-1, TC-2 and TC-8, as well as on the board of the Austrian ESIS group. We thank him for his important contributions to ESIS.
3. Hryhoriy Nykyforchyn is a Professor at the Karpenko Physico-Mechanical Institute of the National Academy of Sciences of the Ukraine. He is being awarded this honor for his outstanding research in the field of corrosion fracture mechanics of structural materials and methods for improving their characteristics for operation in corrosive and hydrogen environments. He has concentrated his attention on the problems of corrosion-hydrogen degradation of structural steels during long-term operation of power plants, refineries, as well as oil and gas trunk pipelines. He is the Chair of the Subcommittee on Hydrogen Degradation of TC-10. For this we thank him a give him this award.

Plans for ECF 20 in Trondheim, Norway in 2014 are in progress. At the end of ECF 19, Zhiliang Zhang will present the plans for that conference. At the banquet on Thursday night, I will be able to announce the location of ECF 21 in 2016.

I wish the participants of ECF 19 fruitful discussions.

Leslie Banks-Sills

WELCOME !



Dear colleagues,

The financial crisis of Europe continues and more and more countries appear to be infected. Even more, the citizens of the European countries have to show solidarity - and we, the members of ESIS, can contribute our part by strengthening our society. We can only achieve this goal by being and remaining credible.

Credibility results from the way we present ourselves as scientists and engineers. Which principles govern our daily work? There is consent about ethics in medicine: physicians have their Hippocratic Oath by which they commit themselves "*to make prescriptions for the benefit of the sick according to my ability and my judgment*". Is there something similar in engineering science? PhD students at the Technical Faculty in Kiel (Germany) have to enter the following commitment when receiving their Doctor degree: "*I commit myself to honour the academic degree which will be awarded to me by the Faculty. I also commit myself to search and avow truth to the best of one's knowledge.*"

There is enough reason to discuss this topic at a time when science and research are increasingly dominated by managerial strategies and criteria of operational efficiency. Are we always honest and impartial when publishing our research results? How much are we spoiled by demands to increase our number of publications and improve our fund-raising? Do we represent good examples and are we honest guides for our students or do we teach them that the means are sanctified by the expected benefit? If you want to read more about "Ethics in Science", I recommend reading the respective contribution by K.H. Schwalbe, A. Ingraffea and D. Lovegrove, and I consider ESIS to be the adequate panel to discuss it.

Credibility also results from the way we adhere to democratic rules within our own society. There have been quarrels over the last months concerning the decision process of granting ESIS awards, which finally lead to a resolution of the Executive Committee to generally waive awards in 2012. The ESIS Council has been asked by e-mail for its support in that action. In order to act as transparent as possible and prevent any emergence of rumours, we document the respective resolution and the voting process in the present Newsletter. This has been a crucial test on the intention to regain and preserve credibility and ESIS has passed it!

In order not to run into similar problems in the future again, we have to establish rules which clearly define the specifications, conditions and procedures of granting awards. There have been such rules, actually, years ago, but the respective document got lost together with many other documents due to discontinuities in the administration and the lack of a permanent secretariat. ESIS lost history and thereby identity. The Executive Committee therefore appreciates a registration in the UK through our Secretary James Marrow.

It is a tradition that the awardees are invited to present a scientific paper. Emmanuel Gdoutos was awarded with the Griffith medal and Jaroslav Pokluda with the Award of Merit in 2010 at the occasion of ECF 18 in Dresden. You will find the papers of Prof. Pokluda and Prof. Gdoutos in the present Newsletter.

Collecting contributions for the Newsletter twice a year is a bit laborious sometimes. Thus I would like to encourage ESIS members to submit contributions on their own initiative, whether it is on problems of fracture mechanics, history of ESIS, national activities, etc. This will support my work and it will help to present us as a vivid society.

Wolfgang Brocks

ESIS Website

www.structuralintegrity.eu

- **become a member of ESIS and take advantage of all the "Members Only" resources on this Web site**
- **register automatically as a Member and pay the fee by PayPal system**
- **obtain your username and password for accessing the private area for downloading EGF-ESIS books and Procedures**
- **exchange new ideas, advancements and documents with the other ESIS Members**

Advantages of being an ESIS member

- participation in TC activities and access to TC documents;
- full on-line access to ESIS procedures;
- full on-line access to former EGF-ESIS books;
- support for ESIS activity.

how to renew?
see page 32 or
www.structuralintegrity.eu

COUNCIL VOTE

Awards 2012

At the ESIS Executive Committee meeting on 7th May, 2012, in Berlin, the ExCo voted unanimously on the following resolution:

"The decisions of the Awards Committee concerning ESIS awards to be given at ECF 19 (Kazan) are not acceptable. The reasons are:

(1) the Awards Committee was not elected by ESIS Council in Dresden and the Awards committee does not have the correct number of members (there are nine instead of the necessary ten),

(2) an insufficient number of nominations were received for the field to be competitive (only one nomination was received for each award),

(3) three out of four of the people who were elected for ESIS awards by the Awards Committee are members of that committee,

(4) some of these people have already received one or two ESIS awards in the past".

The ExCo voted that the best option for ESIS is not to present any ESIS awards at ECF 19 Kazan, and asked the ESIS Council for its support in that action. As allowed by the ESIS Statutes, an email vote was held between 11th May and 7th June 2012 on the proposition to not present any ESIS awards at ECF 19 Kazan.

Passing the proposition required a one-half majority of the votes cast, with one-half of the Council voting in order for it to be quorate. The total number of possible votes on the ESIS Council is 31: these are

- the 16 National Representatives (Austria, Bulgaria, Czech Republic, Germany, Greece, Israel, Italy, Poland, Romania, Russia, Serbia, Spain, Sweden, Switzerland, UK, Ukraine),
- the 12 TC votes (TC1, 2, 3, 4, 5, 6, 8, 9, 10, 11, 12, 24) and
- the 3 ExCo voting members (2 Vice-Presidents and the Secretary).

In total, there were 28 votes cast, with the result:

- for the proposition: 26;
- against: 1 and
- abstain: 1.

Hence the Council agreed on the proposition and there will be no ESIS awards presented at the ECF 19 meeting in Kazan.

Statutes

The ESIS Council also voted by email correspondence on revised ESIS Statutes. The vote opened on 9th May and closed on 15th June. Council had opportunities to comment on and revise the statutes before the vote. A change to statutes requires a quorum of two-thirds of the total number of voting members, and the required majority is two-thirds. The total number of possible votes on the ESIS Council is 31 as above.

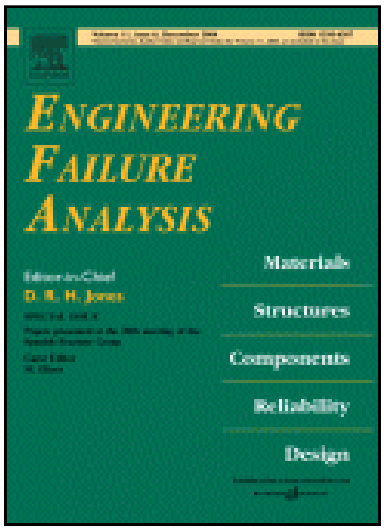
In total, there were 28 votes cast.

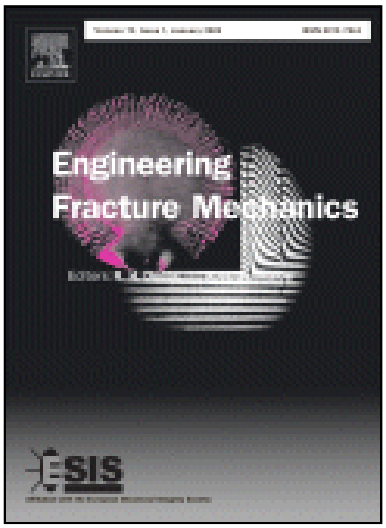
- Those in favor of the new Statutes: 27;
- those opposed: 0 and
- abstain: 1.

The revised statutes were therefore accepted and are published on the ESIS website www.structuralintegrity.eu.

ESIS Secretary: Professor James Marrow

3 Elsevier journals are affiliated with ESIS





TECHNICAL COMMITTEES

TC 1: Elastic Plastic Fracture Mechanics
TC 8: Numerical Methods

ESIS-Workshop on Computational and Experimental Failure Mechanics

ESIS technical committees TC1 (Elastic Plastic Fracture Mechanics) and TC8 (Numerical Methods) held a joint meeting 14/15th June at BAM, Berlin, Germany. Approximately 40 engineers and scientists attended the 2 day meeting. Twenty technical presentations were made over the two days. The themes of the meeting reached from crystal plastic modelling of cleavage and ductile fracture via in situ observation of damage and crack propagation processes to component assessment of pressurized pipes and thin walled structures. A special item of the agenda was a ceremony in honour of Wolfgang Brocks who celebrated his 70th birthday. Prof. Brocks spent many years of his scientific career at BAM.

Prof. Dr.-Ing. H. Yuan

Prof. Dr.-Ing. U. Zerbst

TC 2: Micromechanisms

Report on ESIS TC2/FESI Meeting: Oxford 2-3 April 2012

The 8th meeting of the ESIS TC2 technical committee on Micromechanisms was held at Mansfield College, Oxford University, UK on 2nd-3rd April 2012, in collaboration with the UK Forum for Engineering Structural Integrity (FESI). Over 50 delegates attended: from the UK, Czech Republic, Austria, Slovenia, Germany, France and the Netherlands, with 9 delegates partially supported by ESIS bursaries for young scientists. The organising chairs were James Marrow (University of Oxford) and Jaroslav Pokluda (Brno University of Technology). There were 24 oral presentations and a poster session with over 10 contributions. The meeting sessions, spread over the two days in a continuous programme, were: Microstructure and Plasticity; Fatigue; Fracture and Constraint; and Ceramics and Composites, and were chaired by Jaroslav Pokluda, Peter Flewitt (University of Bristol), Alan Cocks (University of Oxford), David Smith (University of Bristol) and James Marrow.

The topics discussed covered a broad range, with some common themes addressed by several presentations: these included; modelling and measurement of critical shear stress for

plastic deformation; the heterogeneous deformation of polycrystalline grain assemblages responsible for intergranular cracking; the role of constraint and residual stresses on crack tip deformation in fatigue; the influence of microstructural evolution on damage mechanisms and fracture property modelling of heterogeneous microstructures.

The delegates enjoyed a walking tour of Oxford's historical architecture prior to the meeting, and a very convivial candle-lit dinner in the oak-panelled Mansfield College hall; a number of international collaborations may have been sparked off by the event. A special issue of the ESIS affiliated journal, Engineering Fracture Mechanics, is planned for publication in 2013, and will contain papers from the meeting. A delegate list, extended abstracts of all contributions, copies of the majority of the presentations and some photographs of the event are available from the meeting website (http://energy.materials.ox.ac.uk/Meetings/esis-tc2-oxford.html)

Thanks to all those who contributed to a very successful and enjoyable meeting.

T.J. Marrow

Photo: Petr Šesták (Brno University of Technology)

TC 3: Fatigue of Engineering Materials and Structures

ACTIVITIES DURING 2012-2013

(a) Professor Ewald Macha (Opole): Organization of a Summer School on "Multiaxial Fatigue of Materials and Structural Components", held in Poznań, Poland, 26th and 27th June, 2012, which gathered 61 participants. Lectures were delivered by experts employed at Opole University of Technology, Department of Mechanics and Machine Design (this Department belongs to the Centre of Structural Integrity, CESTI, Poland).

(b) Professor Ewald Macha (Opole): Organization of a Special Session on "Multiaxial Fatigue and Fracture" at the 19th European Conference on Fracture – ECF19, to be held in Kazan, Russia, 26th to 31st August, 2012.

(c) Professor Andrea Carpinteri (Parma), Professor Francesco Iacoviello (Cassino), Professor Les P. Pook (Sevenoaks) and Professor Luca Susmel (Sheffield): Chairmen of the 4th International Conference on Crack Paths (CP 2012), to be held in Gaeta, Italy, 19th to 21th September, 2012.

(d) Professor Andrea Carpinteri (Parma), Professor Francesco Iacoviello (Cassino), Professor Les P. Pook (Sevenoaks) and Professor Luca Susmel (Sheffield): Guest Editors of a Special Issue on "Fatigue Crack Paths" of the "International Journal of Fatigue", and Guest Editors of a Special Issue on "Crack Paths" of the International Journal "Engineering Fracture Mechanics", with papers selected from those presented at the 4th International Conference on Crack Paths – CP 2012, to be held in Gaeta, Italy, 19th to 21th September, 2012.

(e) Professor Andrea Carpinteri (Parma), Professor Masao Sakane (Ritsumeikan, Japan) and Professor Shan-Tung Tu (Shanghai, China): Chairmen of the 10th International Conference on Multiaxial Fatigue and Fracture (ICMFF10), to be held in Kyoto, Japan, 3rd to 6th June, 2013.

(f) Professor Andrea Carpinteri (Parma), Professor Masao Sakane (Ritsumeikan, Japan) and Professor Shan-Tung Tu (Shanghai, China): Guest Editors of a Special Issue on "Multiaxial Fatigue Models" of the "International Journal of Fatigue", and Guest Editors of a Special Issue on "Multiaxial Fracture" of the International Journal "Engineering Fracture Mechanics", with papers selected from those presented at the 10th International Conference on Multiaxial Fatigue and Fracture – ICMFF10, to be held in Kyoto, Japan, 3rd to 6th June, 2013.

Professor Andrea Carpinteri

Professor Les P. Pook

TC 4: Polymers and Polymer Composites

NEWS UPDATE 2012

Committee meetings

ESIS TC4 continues to meet twice a year to develop fracture mechanics test methods for

polymers, composites and adhesives and to organise an international conference every three years.

Committee meetings are open to all. Please contact the Eurotel Victoria in Les Diablerets via email <lesdiablerets@eurotel-victoria.ch> to make room bookings. An agenda for the meeting can be obtained from the technical committee secretary, Bamber Blackman (b.blackman@imperial.ac.uk).

Conferences

The 6th ESIS TC4 Int. Conf. on the Fracture of Polymers, Composites and Adhesives took place in September 2011 in Les Diablerets, Switzerland. Selected papers from this conference have been accepted for publication in a special edition of Engineering Fracture Mechanics, to appear in late 2012. See www.tc4pca.elsevier.com. The 7th Int. conference in the series will take place during 14th-18th Sptember 2014.

Active work areas

The following are active work areas, in which the technical committee are developing ESIS TC4 test protocols with the aim that these will become full ISO standands in due course. Anyone wishing to get involved in these exciting work areas should either contact the work area co-ordinator (see below) or the committee technical secretary, Bamber Blackman (b.blackman@imperial.ac.uk) for further details.

1. Polymers:

Following the successful development of standards for slow rate K_c and G_c determination in polymers (ISO 13586-1) and in short fibre composites (ISO 13586-2) and of the develoment of a test standard for these properties at high rates of loading (ISO 17281) and under tension-tension fatigue loading (ISO 15850), the committee is currently developing test protocols in the following areas:

1.1 Work area: J_c testing;

Co-ordinator: Francesco Baldi (baldi@ing.unibs.it)

The committee aims to develop a test protocol to characterise toughness in polymers which fail the LEFM validity criteria for K_c and G_c. A protocol was developed by the committee members Hale and Ramsteiner, based upon a multi-specimen technique. The major limiting factor has proved to be the difficulty to accurately measure the crack growth in the test. Development of the test method is still underway within the committee, with modified test and analysis schemes under consideration. Current round-robin testing is focussing on the use of load-separation criteria techniques.

1.2 Work area: Essential work of fracture;

Co-ordinator: Marta Rink (marta.rink@polimi.it)

The committee aims to develop a plane stress fracture test for polymeric films. A version of the protocol was published in 2001 (*ESIS Publication 28, Chapter 2, Fracture Mechanics Testing Methods for Polymers Adhesives and Composites, Elsevier 2001*) but in the view of the committee, the results produced by this method are currently insufficiently reproducible to warrant standardisation within ISO. The committee is investigating the origins of the poor reproducibility in the results via round-robin studies and additional experimental and theoretical contributions.

1.3 Work area: Determination of G_c via Cutting;

Co-ordinator: Gordon Williams (g.williams@imperial.ac.uk)

The committee aims to develop an alternative technique for the determination of G_c in tough, ductile polymers using a cutting technique. A test protocol has been developed in which a tool is used to remove a thin layer of polymer from a specimen via orthogonal cutting at a constant speed (*Eng Fract Mech 76, (18) p.2711-2730, 2009*). G_c is determined by measuring forces in two directions, in the direction of cutting and transverse to this direction. Two round-robins have now been completed within the committee and recent work has investigated the effects of tool sharpness.

1.4 Work area: Environmenal stress cracking;

Co-ordinator: Leonardo Castellani (leonardo.castellani@versalis.eni.com)

The committee aims to develop a test protocol to determine the sensitivity of different polymers to stress cracking in various hostile environments. The activity started in 2010. The test adopted will follow a fracture mechanics approach and will permit different test environments to be studied. An initial *ESIS TC4 Protocol* has been developed, and round-robin testing is underway using techniques including the buckled plate test, the SENB test and the DCB test.

2. Composites:

Following the successful development of standards for slow rate K_c and G_c determination in short fibre composites (ISO 13586-2) and for delamination resistance of unidirectional laminates in mode I (ISO 15024: 2000), the committee has developed a mode II delamination standard based upon the calibrated end loaded split test (currently ISO CD 15114) and is currently developing test protocols in the following additional areas:

2.1 Work area: Short fibre composites at high loading rates;

Co-ordinator: Andrea Pavan (andrea.pavan@polimi.it)

The committee aims to extend the techniques developed to determine Kc and Gc of short fibre composites at a slow rate (ISO 13586-2) to faster rates (circa 1m/s). Such development will build upon the tecniques developed by the committee for determining K_c and G_c in bulk polymers at higher rates (ISO 17281). Technical issues being addressed include the identification and teatment of 'pop-in' failure, the mitigation of dynamic effects and specimen manufacture and fibre orientation effects.

2.2 Work area: Delamination of UD laminates at high rates;

Co-ordinator: Ian Horsfall (i.horsfall@cranfield.ac.uk)

The committee aims to extend the test developed for the determination of delamination resistance at quasi-static test rates (ISO 15024) to higher rates (circa 1m/s). The challenges include the mitigation of dynamic effects, the measurement of accurate and reliable test data and the treatment of kinetic energy efects. A protocol was drafted by Bamber Blackman and a round-robin using a UD carbon fibre PEEK composite has been completed.

2.3 Work area: Delamination fatigue in UD laminates;

Co-ordinators: Steffen Stelzer (Steffen.Stelzer@unileoben.ac.at)

Andy Brunner (andreas.brunner@empa.ch).

The committee aims to develop a test protocol to measure the fatigue resistance of composites to failure by delamination fatigue. The quasi-static test protocol (**ISO 15024**) has been modified for fatigue loading at constant applied crack opening displacement. Two round robins using a carbon fibre reinforced composites has been completed, and a draft mode I fatigue protocol has been written. In the most recent round-robin, attention has turned to mode II delamination resistance, with the end-loaded split and the end-notched flexure tests both being investigated.

2.4 Work area: Fracture resistance of nano-composites;

Co-ordinator: Gordon Williams (g.williams@imperial.ac.uk)

The committee is investigating the use of standardised LEFM techniques, e.g. ISO 13586, to measure K_{Ic} and G_{Ic} in nano-composites. The aim was to address the reasons for the very different values of K_c and G_c reported in the literature for nominally identical materials. A first round-robin has been completed and the results submitted for publication. The main issue identified has been the notching technique used and these are still currently under evaluation by the committee.

2.5 Work area: Mixed-mode partitioning schemes for laminates;

Co-ordinator: Alojz Ivankovic (alojz.ivankovic@ucd.ie)

The committee has recently resumed work in the area of mixed-mode fracture of composite laminates. In 2011, a numerical round-robin was launched with eleven laboratories participating to investigate mixed-mode partitioning schemes and the effects of damage. The activity is being led by Professor Ivankovic at University College Dublin. This activity has generated considerable interest not just within TC4, but also within the wider fracture community, where the issues surrounding mixed-mode partitioning have remained contentious. The first, multi-stage round-robin is underway.

3. Adhesives:

3.1 Work area: Fracture of structural adhesive joints;

Co-ordinator: Bamber Blackman (b.blackman@imperial.ac.uk)

The committee aims to develop linear elastic fracture mechanics (LEFM) test standards for the determination of G_c in structural adhesive joints under modes I, II and mixed I/II loading regimes. The development of the test protocol for mode I fracture is now complete following the publication of a British Standard in 2001 (BS 7991:2001) and an ISO standard in 2009 (ISO 25217: 2009). The current round robin activities in the committee are directed towards the development of a mode II test using the calibrated end-loaded split (C-ELS) test and in mixed-mode using the fixed-ratio mixed-mode (FRMM) test. There is a future goal to extend the LEFM tests to high rates and to fatigue loading conditions.

3.2 Work area: Peel testing of flexible laminates;

Co-ordinator: Neal Murphy (neal.murphy@ucd.ie)

The committee aims to develop test protocols to determine the adhesive fracture toughness, G_a, for the debonding of a flexible layer by peeling. The central goal has been to develop geometry independent tests where a measurement is made of 'how well a substrate is bonded' as opposed to the much more commonly measured peel strength, i.e. 'how difficult it is to peel the substrate.' Initial round robins focussed on the measurement of adhesion between layers in packaging laminates and more recent activity has been directed towards the peeling of metallic layers bonded by

structural adhesives. The major challenge here is to accurately account for the energy dissipated plastically in the peel arm. The protocol for flexible laminates is now complete, and ready for ISO submission.

Bamber Blackman

TC 6: Ceramics

The TC 6 Ceramics core members organized a meeting during the *12th Conference of the European Ceramic Society* in Stockholm, Sweden 19-23 June 2011.

We decided to change the chair of the TC 6 ceramics as soon as possible but not later than the end of 2012.

We decided to organize the Int. Conf. „Fractography of Advanced Ceramics" in Slovakia in 2013.

In 2011 we started to organize the Symposium "Nanoceramics and Ceramic Based Nanocomposites" in the frame of E-MRS 2012 Fall Meeting, which will take place in Warsaw, Poland, 17 – 21 September 2012, supported by the European Materials Research Society. The Symposium organizers are Ján Dusza, Csaba Balázsi, Witold Łojkowski, Mike. J. Reece and Ralf Riedel.

For more information, to register and to submit an abstract please visit

http://www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=500&Itemid=1

All submissions will be peer-reviewed. The accepted papers will be published in

- Journal of the European Ceramic Society (Impact factor: 2.574)
- Central European Journal of Chemistry (Impact factor: 0.991)

The next meeting of the core members of TC 6 Ceramics will be held during the 10th Int. Symp. on Ceramic Materials and Components for Energy and Environmental Applications, 10th CMCEE, May 20-23, 2012, Dresden, Germany.

Jan Dusza

TC 10: Environmentally Assisted Cracking

Under the auspices of the ESIS TC-10 and organized by the Transport Technology Department of Maritime University of Szczecin, the Conference "Wear Processes 2012" will be held in Świnoujście, Poland, from 12 to 14 of September 2012.

The main topics of the Conference are as follows:

- Fundamental problems of deterioration and wear of materials.
- Simple and complex deterioration processes.
- Hydrogen degradation of materials.
- Wear processes accelerated by hydrogen degradation and corrosion.
- Modeling of wear processes.
- Cases of abnormally rapid of wear.

Selected papers will be published in "Solid State Phenomena"

More details in
http://wear2012.am.szczecin.pl/

J. Toribio

H.M. Nykyforchyn

TC11: High Temperature Mechanical Testing

- Main committee meeting at EDF, Gloucester, Barnwood, UK, on 15th May 2012
- Temperature measurement working group Meeting at CCPI, Sheffield-Rotherham, UK, on 17th July 2012

WORKSHOP ACTIVITIES

TMF-Workshop 2011

The editing of the papers to be published in the International Journal of Fatigue is virtually complete and it is planned that the special issue would be issued later in the year. The editing of the papers to be published in the special issue of Materials at High Temperatures is close to being finished. Information about the TMF Workshop 2005 has been transferred to the website www.tmf-workshop.bam.de. It will be linked with the HTMTC Website www.htmtc.com, too. The CoP for strain controlled TMF testing, originally published in 2006, is beside the standard ISO 12111 one of the most important TMF testing procedure documents worldwide. Thus it has been published again on the TMF-Workshop website because it has been removed from the website at JRC, Petten, NL.

Workshops on Quality Assurance Issues for High Temperature Testing

The 1st workshop took place on 15-16 May 2012 at EDF, Gloucester, Barnwood, UK. 38 participants attended the Workshop. The program contained numerous excellent contributions from experts in the area of quality assurance acquired from institutes, industry and from ESIS TC11 (HTMTC).

It is intended to hold the 2nd Workshop at INCOTEST, Hereford, UK on 13th-14th November 2012.

Joint workshop on Accelerated Testing Methods together with IOM3 High Temperature Materials Committee (HTMC)

Dr Barnard proposed that a meeting on '*Accelerated Testing Methods'* would be a viable venture. The meeting will probably take the format of a 1½ day meeting in spring 2013 possible at the Riverside Centre (Pride Park) Derby. The meeting will comprise three ½ day sessions:

a) Testing Methodology, organised by the HTMTC,

b) Data for Lifing organised by Mike Spindler, EDF and

c) Metallurgical methods, organised by the IOM HTMC.

The Testing Methodology session could include acceleration by stress, temperature & environment. The automotive sector use truncated wave forms and 'rainfall' analysis, mostly in the non-creep regime. P Barnard agreed to pursue the matter and try to confirm that the dates would dovetail in with Wednesday 22nd May 2013**,** the proposed date of the HTMTC Meeting.

Workshop on Non-Contact High Temperature Strain Measurement

Dr. Klingelhöffer contacted Prof Dr Nikbin and Dr Catrin Davies of IC, London, to hold a workshop on non-contacting strain measurement. This topic should contain Digital Image Correlation techniques and non-contact extensometry, too. It is planned to hold the workshop in autumn 2013 at IC, London.

Working party activities

Testing in Controlled Environments
(Convenor: O O'Grady)

The Draft *'Scope & Objectives'* had been prepared. It was agreed that there was merit in pursuing the subject provided the Scope was widened to encompass '*Non-Standard Testing Techniques'* Members of the Working Group would include Owen O'Grady, Phil Jones and Mike Lynch. The Convenor agreed to revise the Scope.

Temperature Measurement for HT Testing
(Convenor M S Loveday)

Mr Loveday reported that he had relocated and re-plotted the data that he had been recorded approximately 15 years ago at NPL showing the results of drift measurements on Type R Pt-Pt/Rh thermocouples after long term creep tests. The implications of thermocouple drift will be incorporated into the Draft CoP. It was also reported the results of further calibrations of thermocouples had been forwarded to Andrew Wisbey, SERCO, who is co-ordinating the Thermocouple Calibration Inter-comparison exercise. Furthermore some additions have been made to the Bibliography for the draft CoP.

Code of practice for stress/load controlled TMF testing

Dr Stephen Brookes (Rolls-Royce-MTOC, Dahlewitz, D) gave a presentation based upon the in house testing procedure developed at the RR-MTOC. The stress controlled TMF tests performed at MTOC are intricate and incorporate a combination of temperature-loading phases replicating the service cycle of a component. The Committee supported the proposal that there was a need for a CoP covering Stress Controlled TMF testing and Dr Brookes offered to provide a document which could provide the basis of a CoP which could be circulated to other interested parties who could form a Working Group. Mr Brooks, NPL, expressed interest and it is thought that representative from Exova, SERCO, Risley, together with some groups in Germany would wish to participate. Dr Brookes agreed to circulate a draft document for circulation to interested parties.

Hellmuth Klingelhöffer

TC 24: Updates 2012

On 30th March 2012 a TC24 Workshop has been hosted in PoliMI - Department of Mech. Engineering, Via La Masa 1, Milan.

The main topic of the meeting was to present the results of a PoliMi project named MARAXIL ('Manufacturing Railway Axles with Improved Lifetime') funded by Regione Lombardia. Within this project, developed in cooperation with IWM-Freiburg (Dr. M. Luke) and LucchiniRS - Lovere, the research has addressed the improvements in propagation lifetime induced by cold rolling.

The presentation of MARAXIL results will also be the opportunity for the 'railway structural integrity' community to meet again after the previous successful TC24 meetings held in Berlin (October 2010) and London (March 2011) and to discuss the advances in researche and other ongoing cooperative projects (WOLAXIM, EURAXLES, SUSTRAIL).

The program of the workshop was:

- Consolidation of a material database for axle crack growth calculations (M. Luke and D. Regazzi, IWM & PoliMI);
- Effect of rolling on axle life prediction (M. Carboni et al., PoliMi and IWM);
- New detection method for axle corrosion (J. Rudlin and A. Raude, TWI);
- Early phase of corrosion-fatigue damage in A1N (S. Beretta & A. Loconte, PoliMi);
- Some aspects of safe-life and damage tolerant design of railway axles (U. Zerbst,

BAM);

- A comparison of SIF calculations for an axle (M. Sander, Rostock Univ.);
- POD and definition of a new calibration sample for axles (PoliMi, LucchiniRS and Gilardoni);
- Discussion on the definition of axle fatigue limits and K_f factor (S. Cervello, LucchiniRS);
- Updates about the ongoing cooperative projects (Euraxles, WOLAXIM, SUSTRAIL and others);
- Closure and visit to MECC@POLIMI Labs together with demonstration activities.

The meeting, that had some 70 participants, has surely confirmed the activity of the 'railway structural integrity community'. The presentations of the meeting are available at the TC24 website: http://esistc24.mecc.polimi.it, where also the presentations of the previous meetings can be found.

Figure 1– One of the presentations at the TC24 meeting

Figure 2 – Demonstration of one of the devices being prepared within the WOLAXIM project.

The next TC24 meeting will be held on 25th October 2012 at TWI (Cambridge, UK) on the occasion of the closure of the EU project WOLAXIM dedicated to new tools for damage and corrosion detection of axles (for more information see TC24 website).

Stefano Beretta

20th European Conference on Fracture

30th June 30 - 4th July, 2014
Trondheim, Norway

http://www.ecf20.no/

CALENDAR OF TC MEETINGS

TC 4	26th-28th September, 2012	Committee Meeting	Les Diaberets, Switzerland	b.blackman@imperial.ac.uk lesdiablerets@eurotel-victoria.ch
TC 4	15th-17th May, 2013	Committee Meeting	Les Diaberets, Switzerland	b.blackman@imperial.ac.uk lesdiablerets@eurotel-victoria.ch
TC 4	September 2013	Committee Meeting	Les Diaberets, Switzerland	b.blackman@imperial.ac.uk lesdiablerets@eurotel-victoria.ch
TC 4	May 2014	Committee Meeting	Les Diaberets, Switzerland	b.blackman@imperial.ac.uk lesdiablerets@eurotel-victoria.ch
TC 4	14th-18th September, 2014	7th Int. ESIS TC4 conference		

TC 11	13th-14th November, 2012	2nd Workshop on Quality Assurance Issues for High Temperature Testing	INCOTEST, Hereford, UK	malcolm.loveday@np.co.uk
TC 24	25th October, 2012	Committee Meeting, closure of the EU project WOLAXIM	TWI Cambridge (UK)	stefano.beretta@polimi.it

PUBLICATION ACTIVITIES

Journal	Title	Source	Editor	Status
Eng Fract Mech	Damage Tolerance of Railway Axles	TC24 meeting in Milan	S. Beretta	EFM 78 / 5, March, 2011
Int J Fatigue	Multiaxial Fatigue Models	ICMFF9 Multiaxial Fatigue	A. Carpinteri L. Pook C.M. Sonsino	IJF 33 / 8, Aug. 2011
Eng Fract Mech	Mesomechanical Modelling of Fatigue and Fracture	TC 8	H. Yuan	EFM 78 / 3, Feb. 2011
Eng Fract Mech	Multiaxial Fracture	ICMFF9 Multiaxial Fatigue	A. Carpinteri L. Pook A. Spagnoli	EFM 78 / 8, May 2011
Int J Fatigue	Physical and Phenomenological Approaches to Fatigue Damage	Colloqium XV-ICMFM TC 3	E. Macha D. Rozumek	IJF 39 / 6, June 2012
Eng Fract Mech	Micro and Macro Cracks	ECF 18	W. Brocks H. Yuan	9 papers accepted, editing process finished
Int J Fatigue	Recent Progress in the Understanding of Fatigue Crack Propagation	ECF 18	H.J. Christ	14 papers accepted, editing process finished
Eng Fract Mech	Fracture of Polymers, Composites and Adhesives	6th Int. ESIS TC4 conference	B.R.K. Blackman J.G. Williams	21 papers submitted. To appear – late 2012
Int J Fatigue	Thermomechanical Fatigue	2nd Int. Workshop on Thermo-mechanical fatigue, May 2011, BAM, Berlin, Germany / TC 11	H. Klingelhöffer	11 papers accepted; end of review in Feb. 2012; expected to appear in 2012
Int J Fatigue		VHCF-5	C. Berger B. Pyttel	selection of contributions
Eng Fract Mech	Micromechanisms of Deformation and Fracture	TC 2 Meetings in Berlin and Oxford	J. Pokluda J. Marrow	peer-review started
Eng Fract Mech		4th Int. Conf. on Crack Paths (CP 2012) / TC 3	A. Carpinteri L. Pook	proposed
Int J Fatigue		4th Int. Conf. on Crack Paths (CP 2012) / TC 3	A. Carpinteri L. Pook	proposed

13th International Conference on Fracture

May 26-31, 2013
Beijing, China

www.icf13.org/

14th International Conference on Fracture

ICF 14

May 7-12, 2017
Rhodes, Greece

Executive Chair:
Professor Emmanuel Gdoutos
egdoutos@civil.duth.ge

Technical Programme Co-Chair:
Prof. James Marrow,
james.marrow@materials.ox.ac.uk

International Steering Committee:
Professor D M R Taplin
coliemore@hotmail.com

CALENDAR OF CONFERENCES

August 26th-31st, 2012	19th European Conf. on Fracture (**ECF 19**)	Kazan, Russia	www.ecf19.ru e-mail: ecf19@acadenergo.ru
August 27th-31st, 2012.	38th Solid Mechanics Conference (**SolMech 2012**),	Warsaw, Poland	http://solmech2012.ippt.gov.pl/
September 3rd -7th, 2012	33rd Risoe Int. Symp. on Materials Science, "Nanometals – Status and Perspective"	DTU, Roskilde, Denmark	http://www.vindenergi.dtu.dk/Conferences/symp33.aspx
September 10th -14th, 2012	6th European Congress on Computational Methods in Applied Sciences and Engineering (**ECCOMAS 2012**)	Vienna, Austria	http://eccomas2012.conf.tuwien.ac.at
September 16th-21st, 2012	9th Int. Conf. on Fatigue Damage of Structural Materials	Hyannis, MA, USA	http://www.fatiguedamageconference.com/index.html
September 19th-21st, 2012	4th Int. Conf. on Crack Paths (**CP 2012**)	Gaeta, Italy	http://www.CP2012.unipr.it
September 27th, 2012	FESI CPD Seminar: Numerical Simulations in Fracture Integrity Management	Imperial College London, UK	e-mail: poul.gosney@fesi.org.uk

November 3rd-4th, 2012	Int. Conf. on Engineering Education and Management Innovation (**ICEEMI 2012**)	Changsha, China	www.iceemi.org
November 7th-9th, 2012	Cellular Materials (**CELLMAT 2012**)	Int. Congress Center Dresden, Germany	www.conventus.de e-mail: anja.kreutzmann@conventus.de
November 9th-15th , 2012	**ASME 2012** Int. Mechanical Engineering Congress	Houston, Texas, USA	imece@asme.org
November 13th-14th, 2012	Int. Workshop on Quality Assurance in Mechanical Testing Laboratories (**QAMTL**)	Inco Test, Hereford, UK	www.htmtc.com
December 3rd-5th, 2012	6th Int. Conf. on Coupled Instabilities in Metal Structures (**CIMS 2012**)	Univ. Strathclyde, Glasgow, UK	http://www.cims2012.org
December 5th-7th, 2012	1st Int. Conf. on Performance-Based and Lifecycle Structural Engineering *(***PLSE 2012***)*	Hong Kong, China	http://www.polyu.edu.hk/fclu/PLSE2012 e-mail: clplse@inet.polyu.edu.hk
Dec. 22nd-23rd, 2012	3rd Int. Conf. on Advances in Materials and Manufacturing Processes (**AMMP 2012**)	Beihai, China	www.icammp.org
March 10th-14th, 2013	8th Int. Conf. on Fracture Mechanics of Concrete and Concrete Structures (**FraMCoS-8**)	Toledo, Spain	http://www.framcos8.org
May 26th –31st, 2013	13th Int. Conf. on Fracture (**ICF13**)	Beijing, China	http://www.icf13.org
May 28th - 29th, 2013	12th Int. Conf. on Engineering Structural Integrity Assessment (**ESIA 12**)	Manchester, UK	www.fesi.org.uk e-mail: fesi@fesi.org.uk
May 29th-31st, 2013	V Int. Conf. on Computational Methods in Marine Engineering (**MARINE 2013**),	Hamburg, Germany	http://congress.cimne.com/marine2013
June 3rd-7th, 2013	Aeronautical Fatigue and Structural Integrity (**ICAF**)	Jerusalem, Israel	e-mail: abrot@iai.co.il
June 12th-14th, 2013	4th Int. Conf. on Computational Methods in Structural Dynamics and Earthquake Engineering (**COMPDYN 2013**)	Island of Kos, Greece	http://www.compdyn2013.org.
June 16th-20th, 2013	11th Int. Conf. on Structural Safety and Reliability (**ICOSSAR 2013**)	Columbia University, New York City, USA	www.civil.columbia.edu/icossar2013
July 1th – 3rd, 2013	7th Int. Conf. on Materials Structure & Micromechanics of Fracture (**MSMF 7)**	Brno, Czech Republic	http://msmf.fme.vutbr.cz
September 9th-13th, 2013	7th Int. Conf. on Low Cycle Fatigue (**LCF7**)	Aachen, Germany	www.lcf7.de
September 25th-27th, 2013	Intelligent Materials	Kiel, Germany	www.intelligent-materials.de

ESIS
Newsletter #50-2012

ETHICS IN SCIENCE

Karl-Heinz Schwalbe, University of Bochum and
Hamburg University of Technology, Germany
Antony Ingraffea, Cornell University, Ithaca, NY, USA
Daniel Lovegrove, Elsevier, Oxford, UK

Short version of presentations at
International Conference APCFS, Busan, Korea, May 13-16, 2012
and at
ICM11, Lago di Como, Italy, 5 – 9 June 2011.
See also
http://issuu.com/dvm_berlin/docs/ethics_in_science?mode=a_p

Introduction

Science publication media are increasingly confronted with problematic paper submissions. This is not only related to authors, not even related only to publication as such, the problem is much wider as we will see later. This communication is based on our own experience in editing and publishing a journal.

What are the Problems?

We as editors of a journal are confronted with ethical problems related to publications, which we start with; comments on more general problems in the area of science will follow.

The problems in scientific publication will be illustrated in the following by a number of typical examples.

Plagiarism

What is of increasing concern is shameless copying of other authors' papers, word by word, page by page, derivation by derivation, to pretend having done original work, and giving the community the false impression that they have done that work. Fortunately, we have numerous knowledgeable reviewers who discover a large number of, but not all, suspicious manuscripts.

Some generic and notorious cases

1. Authors submit the same manuscript to more than one journal. In a recent case an author submitted three copies of his work to three journals. As a consequence, three editors and three groups of reviewers were misused to deal with a single paper.
2. Authors send a manuscript that was rejected by one journal to another one without making the editor aware of the previous rejection. In our opinion, re-submission of a rejected paper to another journal would be acceptable if the previous rejection – preferably together with the reviewers' comments – would be communicated to the new editor, and if the author had made changes reflecting the reviewers' comments, rather than just submitting the paper unchanged.

Two very special cases:

3. A professor *XX* created his own journal and in so doing created an incredibly (and ridiculously) large number of publications and citations. This journal is known as "Prof. *XX's* publication farm".
4. An article in Nature[1] reports a case of misconduct in Zhejiang University (ZJU) in Hangzhou: After the editor of a journal found "….that figures in a manuscript by *He Haibo*, a scientist…..who had been hired by the ZJU only months before, were suspiciously similar to those in an article that He had published elsewhere….. the case, which eventually led to the retraction of eight papers…..Articles attacked the laxity of a system that gave leadership roles to the likes of *Li Lianda,* dean of the department….and *He's* supervisor, who was largely absent from the lab and unfamiliar with the work, but was last author on some of *He's* papers. "There was plagiarism, fabrication and falsification….." says *Yang Wei…..",* president of the university. Wei has set up measures for preventing scientific misconduct at his university.

Basically, we see two kinds of plagiarism:

- Authors copy other authors' work, without citation of the original publication. This is "classical" plagiarism;

[1] *David Cyranoski*, A University Cracks Down on Misconduct in China; Nature, 481, 12 January 2012, pp 134-136.

- Authors copy their own work; we call this "paper recycling" or "self-plagiarism".

The first case is simply theft or fraud. The author steels other peoples' (intellectual) property. Here, copyright problems with probable legal prosecution can be the consequence. It is a common belief that science is based on trust and honesty; neglecting these virtues – if discovered – may lead to denial of an academic grade, e.g. a doctoral degree, publication of a notice in the journal telling the community what has happened or, in extreme cases, the journal editor refusing to consider that author's work for a set period of time.

A very prominent case has surfaced in Germany: The former defense minister, *zu Guttenberg,* was accused of having used other authors' work without citation for his PhD thesis. Consequently, he lost his PhD Degree. Some additional prominent figures in Germany were also denied their PhD title. One of the reasons for this development is that many professors decorate themselves with a large number of PhD students whom they never can supervise, which is certainly not supporting the quality of research. This is good for people who just want the doctoral title for their business cards and name plates, whereas the ideal motivation for PhD study should be the start of a scientific career. An easy way of receiving a scientific degree or title is buying it. There are agencies selling Dr. Degrees and Professor Titles having their origin in remote countries[2]. Although these "upgrades" have no real value, they are worth the money (up to € 40.000) because the risk of being discovered is low. Here formal decoration for the ego is the driving force.

These and similar incidents represent just the end of a chain. The reasons for this kind of behaviour can be seen in pressure exerted by the scientific system and also in the authors' excessive ambition to have a long list of publications – "The more the better" - , see example #3.

Consequently, the total number of publications and also the number of journals are rapidly increasing. Like somebody wrote to us: "I guess this is why I stopped reading the journals, too much bulk and nothing of value. Maybe I am seeing this differently, but I guess quantity rules over value."

There are editors who try to push up the impact factor of their journals with unfair means, for example: They require from their authors to cite papers of their own journal.

Authorship

Authorship is also a key item in scientific publication. Consequently, often too many researchers are listed as authors although they had not been involved in the investigation reported in the publication. Frequently heads of research groups insist on being listed as authors, "strategic authorship", without having contributed to the research work. Ideally, authorship – including the order of authors – should strictly follow the amount of contribution to the work described in the paper. We know of leaders of research groups, who do not just want to be co-authors, they want to be the first author. Their concern seems to be that they tend to disappear from the radar screens of their peers in the scene if they do not show up as authors or – better – as primary authors. This is certainly unfair against the people, who do the hard work, but: If a professor's researchers are successful, then the sun shines also upon him or her, doesn't it? Notwithstanding these arguments, a group leader may become co-author if he or she has substantially contributed to the substance of the work being published.

Finally, it has to be made clear that every author has the right and the duty to check the manuscript before it goes to the journal.

Reviewing manuscripts

We have a further problem that seems to be ever worsening, and this is related to reviewing manuscripts. Until a few years ago, the complete review process was done by paper mail. When a manuscript arrived, the secretary made two copies, and we sent these copies to experts who we believed would be willing and able to review the paper. Usually, we got back two reviews, mostly by the deadline. This has completely changed, to the dismay of authors, editors and experts who are asked to do reviews. We make the following observations:

1. An expert does not respond to the invitation, even after a reminder.
2. After a while, an expert responds after a reminder, this could be negative or positive.
3. If negative, the expert is expected to name a person (with e-mail address) who may be able to do the review; however, frequently this does not happen.
4. If the response is positive, then it happens that the reviewer does not deliver his/her comments by the deadline. Then we send a reminder. Then there are again two options:
   - 4.1 No response by the new deadline, sometimes even no response after the second reminder. Or:
   - 4.2 The review will be delivered.

This process can be extremely time-consuming, and after a while we receive letters from authors

[2] DIE ZEIT, No.20, 10 May 2012.

who are very disappointed by the slow review process.

We are now approaching at least four, sometimes even more experts, hoping that we receive at least two, better three, useful reviews. It is clear to us that the work load of those people who are able do to a decent review can be extremely high; the work to be done just to keep their groups going basically does not allow any additional actions.

It happens that *reviewers recommend that the author adds publications of the reviewer to the author's references*. This is another kind of misconduct owing to the pressure of having high scores in citations.

Education

The contemporary study system in Germany and the US has become extremely pressing. Every course a student applies to is a contribution to the examinations; the student has to pass an exam, even if he/she wishes to attend just for personal interest. Students just compete for credit points, again a stupid formalization in the science system. There is little time for widening a student's horizon beyond his/her major study, not even during the semester holidays when exams have to be prepared and passed. Creativity and motivation cannot develop under these circumstances. Our students are now approaching what employees in industry sometimes are: Robots made for a specific purpose. In Germany, about 70% of the students have financial trouble, and the high work load in the university makes it almost impossible to earn some money by short term jobs. In the U.S., the guarantee of federal government loans for students has become a contentious economic and political issue. Between 40 to 50% of German students report difficulties with the new Bachelor degree system. Depression and fear of exams are abundant; the need for psychological treatment is the consequence.

We should bear in mind that *we are stealing* the most important property of a young person: *his or her youth*. We will have to pay for it.

Costs of Research Misconduct[3]

An aspect that is usually not in our focus is possible harm to public health. Due to the importance that goes far beyond just misconduct, we extract some details from the report "iThenticate" cited in the footnote. It provides a very detailed analysis on the costs of misconduct in science.

Costs for the individual may consist in loss of job, revoked awards, lawsuit, and last but not least in questioned integrity. The publishing media may see its reputation damaged and loss of excellent authors as well as of sales figures.

We cite a complete paragraph from iThenticate: "The Public Library of Science journal, *PLoS Medicine*, published a study, titled 'The Costs and Underappreciated Consequences of Research Misconduct: a Case Study,' which quantified the costs of misconduct. Utilizing a "data-based modeling approach" and applying it to a real example of scientific fraud, *PLoS* researchers were able to calculate actual dollar amounts for the damages incurred. In the end, they determined that their experimental case directly cost the university involved $525,000. This amount included costs for case deliberation, an inquiry panel, as well as the use of an investigation committee, comprised of eight individuals. However, this calculation may be conservative because it does not include several other indirect costs. Taking their statistical model one step further, while also employing external sources to determine the national extent of institutional misconduct, the *PLoS* group calculated that *"the direct costs would exceed $110 million" for the United States in 2010 alone.* Given the data for increased misconduct over the past few years, this number will likely be significantly higher in 2012.

A prominent case of misconduct involved anesthesiologist Dr. Scott Reuben, who was exposed in 2009 for having fabricated at least 21 papers. The prominent medical journal *Anesthesia & Analgesia* had published 10 of Reuben's papers, and even though the materials were later retracted, the damage was already done. The editor-in-chief of *Anesthesia & Analgesia* highlighted the cost of misconduct in this case:

"We are talking about millions of patients worldwide, where postoperative pain management has been affected by the research findings of Dr. Reuben." [16][4] Beyond directly affecting the health outcomes for the general public, misconduct also works to turn back the clock on progress within the research community. Time spent on research based on fraudulent work is wasted effort. Moreover, fraudulent or falsified research can be passed on and used by other researchers, even post retraction.

According to a report of the *British Medical Journal*[5], financial ties between pharmaceutical

[3] http://www.ithenticate.com/

[4] Citation in iThenticate

[5] VERONICA YANK, DRUMMOND RENNIE, LISA A BERO, Financial ties and concordance between results

companies and publications have been discovered.[6] "….. A high and increasing proportion of biomedical researchers have financial ties to the pharmaceutical industry.[1-5] (*The superscripts in these excerpts refer to references in the original report.)* Such researchers are more likely to publish articles—economic analyses, reviews, opinion pieces, and even randomised controlled trials—that support products produced by the industry.[4 6-12] Editors and journals also have been criticised for having financial conflicts of interest that may favour drug companies. Meta-analyses published up to December 2004 that were not duplicates and evaluated the effects of antihypertensive drugs compared with any comparator on clinical end points in adults…..*124 meta-analyses* were included in the study, *49 (40%)* of which had financial ties to one drug company…… Some *antihypertensive drugs* have been shown to *dramatically improve mortality and morbidity. The market* for these and other antihypertensive drugs *is highly* competitive and *lucrative*. According to market research, both angiotensin receptor blockers and calcium channel blockers were in the top 10 list of global therapeutic drug classes by sales in 2005, equating to earnings of over $26b (£13b; €18b).[23] Concern exists about the effect of such profits on doctors. ….. We included meta-analyses published up to December 2004 that evaluated the effects of antihypertensive drugs on clinical outcomes in adults……*Our findings have considerable relevance to the real world, however, as the marketing of antihypertensive drugs constitutes a multibillion dollar a year industry*, and antihypertensives are some of the most prescribed drug classes in the world….. Our study also exposes a *failure of peer review*. Both editors and peer reviewers must have read manuscript versions of those meta-analyses containing discordant results and

We believe that these kinds of misconduct have to be regarded as a severe scandal, if not crime, which ought to be prosecuted.

Where Do the Problems Come from?

Lack of Awareness of the Problem

Sometimes we receive problematic manuscripts from young authors, e.g. PhD students or post docs, who may not be aware that they do something wrong when they copy from other publications. The cover letter may start with: "I am a student, and I wish to submit....." Our impression is that the younger generation is not aware of problems related to intellectual property or copyright. For example, illegal downloading of music is not considered illegal; it is rather considered a sort of sport. It seems to us that these authors work either without a supervisor or have a supervisor who has no experience with the international publication system.

The generation issue is also related to the easy access to the internet, and everything in the internet is not only available, but it also seems to be there for free. "Copy and paste" is the tool people are used to. The easy access to the world's knowledge is enticing; incorporation into the surfer's work is just a copy and paste step away. Moreover, there is an increasing tendency towards "freedom of information", that is interpreted as "including everything". However, *freely available* information does *not* mean that this information is also *freely reusable!*

The foregoing comments do not mean that we want to discourage inexperienced young scientists to go public internationally; we rather wish to motivate the younger generation to expose themselves to the scientific community; however, they must seek guidance by experienced scientists to avoid disappointments.

The cases described herein reveal a deeper problem, namely:

False Incentives and other Flaws in the Contemporary Science System

In Germany, for example, the salaries of professors[7] and allocation of research funds may depend on the number of PhD students. And many professors decorate themselves with a large number of PhD students whom they never can supervise. This is one of the causes of *people* who just *want* the *doctor title for their business cards and name plates*, whereas the ideal motivation for a PhD study should be the start of a scientific career.

In this context it is worth to note that *Dr. Degrees and Prof. Titles can be bought* with money[8], without the year-long stress of doing serious research work. These degrees and titles come primarily from universities in remote countries, with fees up to € 40.000. The titles are worthless, because there is nothing behind them. They raise the ego of people who need such formal decoration. The deal is worth the money since the probability of being discovered

and conclusions in meta-analyses: retrospective cohort study, BMJ 2007;:39376.447211.BE

6 The order of the cited excerpts from the study has been changed by the present authors for better legibility.

7 This has now been criticized by the German Constitutional Court.

8 EGMONT KOCH, The Title Dealer, Sueddeutsche Zeitung, 10 May 2012 (in German)

is low. This example shows again the greed for more and a lack of shamelessness.

A further point that is worth to observe is related to the conferment of medals and awards. The formalities of proposing candidates and finally selecting awardees should guarantee that this process is as open as possible to avoid closed-circle/insider deals.

We have heard of universities which let jobless people work in their labs; these people receive unemployment pay and are hence cheap lab slaves. This is the negative aspect. A positive aspect is that jobless academics have a chance to work in their field and improve their skills.

During a recent conference it was said during the discussion of a presentation that the president of a prestigious American university let professors know that it is the number of publications, not the content that counts – we guess this is not an exception. Along the same line is the pressure on researchers in universities and research centers to publish a certain number of papers and to acquire a certain amount of funding. And universities are increasingly being organized according to enterprises, where totally different criteria are present. *The outcome of research is ranked by numbers rather than scientific quality;* bean counting is the evaluation tool. We suspect that apart from primitive economic thinking in an area where it does not make much sense, there is a loss of trust in those people who were hired after a thorough procedure for performing high quality research. Universities and other research institutions are increasingly being organized like enterprises, where totally different criteria apply. And the science administrations have become too bureaucratic and believe that "control is better than belief", where "control" means very formal evaluation simply because everybody is able to understand numbers – even bureaucrats remote from science. This has also to do with CEOs of research institutions who came from the world of economy.

Hence: *Evaluations* have become more and more formal and *put* increasingly *quantity before quality*, for example: Acquired money from outside sources; number of publications; number of citations; magnitude of the h-index; number of invited lectures; number of PhD students; number of visiting scientists. In some countries, authors are awarded money for each paper they publish in an established journal.

From a letter we received: "…..In (name of the country withheld), we face a phenomenon much worse than plagiarism. As a matter of fact, publications are not important to receive grants and research funds (therefore, plagiarism is not needed!!), since pseudo-political Committees deliver grants, academic positions and research funds to 'their favourite' candidates, even if such candidates are not the best ones…"

There are obviously aspects of the contemporary science system that we consider devastating to good scientific practice.

We do not want to belittle plagiarism but we put part of the blame on our system of *evaluation of science. In our view, it has become partly perverse*. This may be due to the actual "culture" exerting pressure for speeding up everything we deal with – pressure for "efficiency", yet nobody has ever been able to explain how "efficiency" can enhance creativity - the main raw material of scientific research. As it was pointed out above, evaluations "count beans", look at figures, such as number of publications per year, amount of money acquired from sources outside the university, number of visiting scientists per year (A concrete example: "What, you did not have a single visiting scientist last year? It seems that your group is not sufficiently attractive."), number of PhD theses finished per year, and so on. The submission and evaluation system not only requires a substantial amount of time and efforts, it has also brought about a kind of bureaucracy suppressing science and teaching. Science is being undertaken to satisfy formal requirements, and every system can be satisfied, which was clearly visible in the previous system of "socialism" in Eastern Europe.

Another example of the hype in the belief in numbers: A high impact factor of a journal is believed to be the highest goal to be achieved, because it is supposed to be the prime measure of the quality of a journal. In order to raise this factor, some editors "ask" their authors to cite more papers from their own journal. Besides this being very unethical behaviour, the impact factor is certainly not the only measure of the influence of a journal: We have several more application oriented journals having much influence in technology; however, in these areas the readership is more likely to apply literature to their engineering work, rather than publishing which does not result in citations. On a recent editor conference, one of the present authors (KHS) asked the audience who believes that the impact factor is the prime measure of a journal's quality. About two handfuls out of about 100 editors present raised their hands.

This formal kind of evaluation is counter-productive. Under these circumstances, celebrities such as Albert Einstein, Max Planck, Edwin Hubble and the likes could never have been successful and revolutionize our perception of the world!

Fortunately, this situation is being increasingly recognised; for example, the German Science Foundation (DFG) – when you apply for a grant - wants to see only five publications, those you believe are your most important ones. In the U.S., the National Science Foundation asks for

the same number most related to the proposed work. This means that it is not the length of the publication list that counts but the quality the applicant believes to have achieved. This may have a positive effect on reducing tsunamis of publications. The point is, if you are sufficiently creative you can serve every system. But then creativity is misused for optimising yourself for a system that has to be questioned instead of being used for your research work.

Recently, a group of German professors published a manifesto which identified structural problems behind the scientific system These problems were identified as the excessive pressure for publishing[9] (*publish or perish*), rapid economization of academic institutions (*business management rather than scientific leadership*), high pressure on acquisition of outside money, as well as the requirement to make scientific results publically "attractive" by using sales and marketing instruments from the business world.

In conclusion, the science system needs a strategy for deceleration in order to provide researchers with the freedom for critical reflection. From this requirement, a number of suggestions were derived, and presented in the next section.

Concluding Remarks

So far we have been talking about problematic cases in science and scientific publishing. However, major cases of abuse in science are thankfully rare, and the scientific community as a whole should not be treated as hostages; a 100% screening of everything would be overkill. The supervisors and colleagues should trust their students and colleagues. Anything else creates an atmosphere of mistrust and control.

We see this situation also in a broader context. Calling for more control, stricter laws, and tighter regulations happens in all areas of society. *Life is being made a legal case, subject to steadily increasing observation by authorities of various kinds*.

We need a *balance* between the trust that our colleagues are honest, and attention if there is a hint that something is not o.k. *No 100% control, please!*

Communications on this presentation should be sent to karl-heinz.schwalbe@web.de.

[9] Comments in parentheses by present authors

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THEORETICAL STRENGTH OF SOLIDS: A BRIDGE FROM INTERATOMIC BONDS TO LOCAL PLASTICITY AND FRACTURE

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INTRODUCTION

Theoretical strength (TS) of a perfect crystal of particular chemical composition, also referred to as ideal strength, represents an upper strength limit. TS was usually evaluated only for several special cases of loading, each defined by a single value of the stress tensor component: the uniaxial tension (σ_{ut}) and compression (σ_{uc}), the hydrostatic tension (σ_{ht}) and compression (σ_{hc}) and the pure shear (τ_s). Almost 100 years ago, Polanyi [1] and Frenkel [2] published first calculations of σ_{ut} and τ_s values, respectively. While the Frenkel´s estimation proved to be almost accurate, those of Polanyi and Orowan [3] turned out to be several times higher when compared to recent experimental and even theoretical results [4]. It should be emphasized that theoretical and experimental data on σ_{ut} started to mutually approach only after utilization of ab initio (first principles) calculations including analyses of crystal stability [4]. The ab initio methods are based on computations of electronic structure using the density functional theory and, nowadays, they represent the most precise tool for determination of changes in the total energy of crystals during their deformation. Such obtained energy-strain characteristics are also used as benchmarks for construction of sophisticated semi-empirical interatomic potentials employed in molecular dynamics (MD) studies. In general, the ab initio calculated mechanical characteristics of perfect crystals start to be widely applied in multiscale models of fracture processes of engineering materials.

Scientific and practical significance of TS data lies in several general aspects [4, 5]. These data give us upper benchmarks when improving the strength of advanced materials. They play a decisive role in the fundamental theory of fracture: the stress necessary for both homogeneous (lattice) and heterogeneous (grain boundary) nucleation of dislocations can be well identified with τ_s and the local stress for nucleation of cleavage cracks should overcome σ_{ut}. The ratio σ_{ut}/τ_s reflects brittleness/ductility response of the crystal matrix and the difference in mechanical behavior of perfect and real crystals enables us to clearly separate the role of crystal defects from that of the perfect matrix. During the last 15 years, systematic ab initio computations of multiaxial TS brought results important for many case studies as nanoindentation tests (e.g., [6, 7], emissions of dislocations from grain boundaries (e.g., [8]) or synergy effects in nanocomposites [9]. The fracture energy of special grain boundaries weakened by hydrogen or segregated impurity elements can also be determined using ab initio methods (e.g., [10, 11]).

RECENT CALCULATIONS OF THEORETICAL STRENGTH

When considering a perfect crystal deforming homogeneously in a nonlinear elastic way, the total internal energy of the crystal can be expanded as

$$E = E_0 + V\sum_i \sigma_i\eta_i + \frac{1}{2}V\sum_i\sum_j C_{ij}\eta_i\eta_j + O(\eta^3), \quad i,j = 1,2,...,6, \qquad (1)$$

where σ_i are components of the stress tensor, η_i are components of the Lagrangian strain tensor, C_{ij} are the second order elastic coefficients and V is the crystal volume [12]. Here, the simple Voigt notation can be used since the tensors σ_{ij}, η_{ij} and C_{ijkl} (i,j,k,l = 1,2,3) are symmetric with respect to $(ij) \leftrightarrow (ji)$ interchange. By setting E_0 = 0 and using the internal energy per volume unit $E_u=E/V$, one can simply write

$$\sigma_i = \frac{\partial E_u}{\partial \eta_i}, \quad C_{ij} = \frac{\partial^2 E_u}{\partial\eta_i\partial\eta_j}. \qquad (2)$$

For a prescribed deformation path, the related energy-strain curve can be determined using semi-empirical interatomic potentials or ab initio. Up to 1980, the value of TS for this path was generally assumed to correspond to the maximal stress that is associated with so called volumetric instability related to the point of inflexion on the strain-energy curve (1). However, it turned out that the volumetric instability is often preceded by phonon-induced instabilities. Particularly in the case of uniaxial tension, therefore, the values of σ_{ut} revealed to be much lower than those computed from the inflexion point. This is, however, not the case of a pure shear deformation and the value of τ_s. Therefore, the classical Frenkel´s formula for τ_s can still be used for approximate assessments of τ_s [13, 14].

If the solid is infinitesimally strained from a reference state associated with σ_{ij} by the strain tensor ε_{ij} (in the standard notation), the related Cauchy (true) stress t_{ij} can be expressed as

$$t_{ij} = \sigma_{ij} + B_{ijkl}\varepsilon_{kl}\,, \tag{3}$$

where

$$B_{ijk} = C_{ijkl} + \tfrac{1}{2}\left(\delta_{ik}\sigma_{jl} + \delta_{jk}\sigma_{il} + \delta_{il}\sigma_{jk} + \right. \\ \left. + \delta_{jl}\sigma_{ik} - 2\delta_{kl}\sigma_{ij}\right) \tag{4}$$

is the elastic stiffness matrix ($i,j,k.l$ = 1,2,3), generally asymmetric towards $(ij) \leftrightarrow (ji)$ interchange. Construction of this matrix is crucial for the elastic stability assessment. Namely, the system can be considered to be stable when

$$\det|\mathbf{B}| > 0 \tag{5}$$

during the loading [12, 15], i.e., the elastic stiffness matrix is positive definite. This leads to a set of so called elastic stability conditions that depend on both the crystal symmetry and the applied loading [12]. For cubic crystals under isotropic loading, e.g., the number of resulting stability conditions is reduced to the following three:

$$C_{11} + 2C_{12} > 0; \tag{6}$$

$$C_{11} - C_{12} > 0; \tag{7}$$

$$C_{44} > 0. \tag{8}$$

The first condition is equivalent to the requirement that the bulk modulus is positive (the volumetric stability). The other two conditions are related to the tetragonal and the trigonal shear moduli. The crystal becomes unstable if any of them vanishes. In eqs. (6 - 8), the values of elastic moduli must be determined for a sufficient number of points on the deformation path by introducing a given number of independent small strain deviations. Therefore, the assessment of elastic stability is very demanding and was performed only for a small number of crystals and loading modes [16 - 19]. However, one can also obtain sufficiently precise results when using a much easier method proposed in [20]. In this way, values of σ_{ut} for many fcc and bcc crystals more close to experimental ones were already obtained (see hereafter).

In fact, the elastic instability conditions represent a long wavelength limit (for vanishing wavevectors $q \rightarrow 0$) of a more general instability related to an occurrence of so called soft phonons carrying negative energy in the crystal lattice. Since the phonon energy is related to its frequency ω, the general stability criterion (in the harmonic approximation) requires

$$\omega^2(q,s) > 0 \tag{9}$$

for all wavevectors q and modes s (optical/ acoustic, longitudinal/transverse) [21]. Thus, the soft phonons with finite wave lengths ($q > 0$) may also lead to a crystal collapse. However, such instabilities can be discovered only when computing the phonon spectrum of a particular crystal during deformation and identifying the soft phonons with imaginary frequencies. Up to now, such a complete assessment of phonon-based instabilities was reported in a few works only (e.g. [22, 23]). In these works, the occurrence of some soft phonons with finite wave lengths did not reveal any dramatic reduction of σ_{ut} values with respect to those obtained by the analysis of elastic stability conditions.

Values of σ_{ht}, σ_{ut} and τ_s computed for selected crystals of elements from first principles [4, 24-29] are collected in Tab. 1 along with available experimental data [7, 30-32] obtained on whiskers, nanopillars or from nanoindentation tests. The bold print highlights values for σ_{ut} and σ_{ht} that were achieved by taking the stability conditions into account and those for τ_s obtained by a full relaxation of atomic positions during deformation. All these values agree with experimental ones within a factor of two. Note that, especially for σ_{ut}, one cannot expect a full agreement between theory and experiment since on can hardly avoid some imperfections of specimens (surface roughness, defects) as well as of the loading path. The fcc crystals exhibit the lowest values of σ_{ut} for <110> loading direction and the highest ones for <100> direction. On the other hand, the highest tensile strength of bcc crystals corresponds to <110> and the lowest one to <100> directions. This behavior can be understood in terms of displacive phase transformations [33]. For example, the bcc structure of crystals deformed in the trigonal <111> direction transforms to the simple cubic structure of a relatively high energy. On the other hand, the deformation along the <100> direction leads to the fcc structure of much lower energy that induces the low <100> value of σ_{ut}. This is the intrinsic reason why, at low temperatures, the real bcc polycrystals exhibit brittle (cleavage) fracture along {100} planes perpendicular to <100> direction.

Table 1. Calculated and experimental values of theoretical strength for isotropic, uniaxial and shear loading

Crystal	σ_{ht} [GPa]	σ_{ut} [GPa]		τ_s [GPa]	
	theory	**theory**	**experiment**	**theory**	**experiment**
C (dia)	**88.5**	95<111> 130<100>	20.7 (graphite) 19.6 (graphite)	96.6 <112>	
W (bcc)	57.4	**32.4 <110>** 37.5 <111> 28.9 <100>	**28.3 <110>**	17.5 {110} 17.1 {112}	
Mo (bcc)	42.7	**31.9 <110>** 28.4 <111> 28.3 <100>	**19.8 <110>**	15.1 {110} 14.8 {112}	
Ni (fcc)	**29.0**	**18.3 <100>** **15.4 <111>** **9.1 <110>**		**5.05 <112>**	**5.4 <112>**
Fe (bcc)	**26.7**	27.7 <111> 33.0 <110> 14.2 <100>	13.1 <111>	6.0 {112}	3.56 <111>
Cu (fcc)	**20.2**	**4.6 <110>** **9.3 <100>** **7.5 <111>**	1.59 <110> 1.74 <100> 2.94 <111>	**2.16 <112>**	**1.65 <112>**
Si (dia)	15.5	26.3 <100>	4.14	8.6 <112>	
Ag (fcc)	**11.4**	12.3 <100>	3.80<100>	1.65 <112>	0.71 <011>
Al (fcc)	**11.0** **10.2**	**4.5 <110>** **9.0 <100>** **8.8 <111>**	2.3 (bending)	3.77 <110> 2.84 <112>	
Na (bcc)	**2.2**	0.90 <111> 0.04 <100> 0.20 <110>		0.20 <111>	

After 2000, the influence of coupling of various stress tensor components on TS started to be systematically studied. Tensile and compressive tests of many cubic crystals were simulated in the <100>, <110> and <111> loading directions under superimposed biaxial transverse stresses [33-35]. The maximum tensile stresses were found to be almost linearly increasing (decreasing) functions of tensile (compressive) biaxial stresses for most of the studied crystals. This means that, as a rule, the highest strength of perfect crystals can usually be achieved under the isotropic tensile loading. Results concerning the dependence of the ultimate strain ε_u (at the inflection point) on the applied biaxial transverse stress revealed that, in general, the ultimate strain of fcc metals decreased with increasing biaxial stress whereas the opposite trend referred to bcc metals. The average ductility of fcc metals was higher than that of bcc crystals but, rather surprisingly, it was comparable to that of diamond crystals. Such a response of perfect crystals to the triaxial stress state is qualitatively different from that of engineering materials. In the latter case, an increase in the tensile traxiality always leads to a decrease of ultimate strain which can be attributed to a plasticity driven growth and coalescence of microvoids initiated by secondary phase particles [4]. On the other hand, an assessment of brittleness/ductility behavior of perfect crystals on the basis of the ratio σ_{ht} /τ_s qualitatively corresponds to behavior of both single crystals and polycrystals containing defects. Consequently, this kind of behavior is, at least partially, predetermined by intrinsic properties of the crystal lattice [4].

Values of τ_s were evaluated as a function of the resolved normal stress σ_n on the shear plane while all other stress tensor components were relaxed [36-40]. It was found that the function τ_s (σ_n) increases (decreases) with the applied compressive (tensile) stress practically for all studied fcc and bcc metallic crystals. This is, most probably related to the related variation of friction on shear planes as also discussed in terms of a distribution of valence electron density [39]. However, the ceramic crystals often exhibit an opposite behaviour [41] which means that the strength of interatomic bonds in the shear plane also plays an important role.

Since the results of ab initio calculations stand only for zero absolute temperature, let us briefly mention the influence of temperature on TS. Historically, two relevant methods were applied to predict the temperature influence: the Einstein model of harmonic oscillators combined with the elastic instability criterion and the model of dislocation nucleation supported by phonon fluctuations [7]. These approaches predicted a small drop in σ_{ut} (less than ten of percent) when increasing the temperature from zero to 300K. More recently, both MD simulations of shear TS in Cu and Al [10] and ab initio calculations, corrected for soft phonons with vanishing wavevectors [42], also confirmed the less than 10% difference between the TS values corresponding to 0K and 300K. However, the most physically justified approach to the temperature problem would be so called ab-initio based correlated electron-ion dynamics that is currently under development [43].

FROM INTERATOMIC BONDS TO LOCAL PLASTICITY AND FRACTURE

Nanoindentation tests became a very promising experimental method for identification of ideal shear strength. Due to a very small penetration depth, the stressed volume beneath the sharp nanoindenter is usually constricted to one grain and may be free of pre-existing dislocations. During the nanoindentation, therefore, the increasing local shear stress can reach the value of ideal shear strength to nucleate dislocations in a perfect crystal lattice. Such an onset of local plastic deformation could be detected as a pop-in on the load-displacement curve (e.g., [44]). During the last 10 years, several physically plausible models of the nanoindentation test were published and applied to Mo, W, Cu and Ni crystals (e.g., [6, 7, 31, 45]). These models utilized multiscale "bottom-up" approaches, starting from ab initio calculations of the dependence of ideal shear strength on superimposed normal stress components. The values of indentation forces and penetration depths corresponding to pop-ins could be predicted in a reasonable agreement (± 20 %) with experimental data for all investigated crystals.

The close relation of the function τ_s (σ_n) to dislocation nucleation processes in copper and aluminium was also confirmed by MD simulations [8, 46]. Indeed, the shear stress required for dislocation nucleation in single crystals increased as the resolved normal stress σ_n decreased in the same manner as determined for τ_s. The tensile stress σ_{GB} required to dislocation nucleation at grain boundaries must be linked to both the grain boundary structure and the inclination angle Φ that refers to the degree of rotation of the boundary plane from the coherent twin about the <110> tilt axis. For Σ3 boundaries with $\Phi \sim 45°$ in Cu and $\Phi \sim 30°$ in Al, the dislocations are nucleated and emitted under a relatively low nucleation stresses $\sigma_{GB,Cu} \approx 5$ GPa and $\sigma_{GB,Al} \approx 4$ GPa, respectively. This nearly corresponds to the nucleation resolved shear stress $\tau_{GB} \sim 3$ GPa very close to τ_s of both Al and Cu crystals.

Uniaxial tensile tests of perfect nanocomposites with Mo and V matrixes as function of atomic fraction of reinforced W-fibres was simulated by ab initio methods [9]. The values of σ_{ut} for composites containing about 75% of W were found to be comparable to (or even slightly higher than) that of the 100% W fibre. This synergy effect, significantly beyond the linear mixture rule, could basically be explained by an influence of internal stresses developing in both composite constituents during deformation. In particular, the strength of Mo and V matrixes increased under increasing transverse tensile stresses. Most probably, a redistribution of valence electrons along W-Mo and W-V interfaces also contributed to this effect.

Brittle fracture induced by segregation of impurity elements to grain boundaries is a very important practical problem. Although direct ab initio computations of strength of embrittled boundaries are still in an embryonic state, concepts based on the ideal fracture (surface) energy γ or ideal binding (cohesive) energy U are well in progress. Let us first mention a relationship between the binding energy of a perfectly brittle crystal and its fracture toughness:

$$K_{Ic} \approx \left(\frac{EU}{2S}\right)^{1/2}, \qquad (10)$$

where E is the Young´s modulus and S is the area per atom on the fracture surface [4]. This relation directly connects quantities related to atomistic and macroscopic scales and provides, under the assumption of ideal cleavage fracture, a physical lower-bound benchmark for fracture toughness of engineering materials: $K_{Ic} \in (0.5,1)$ MPa.m$^{1/2}$. Indeed, for most metallic and ceramic crystals, the values of U and S are in units of eV/atom and 10^{-19} m^2/atom, respectively.

There are basically four different atomistic models of impurity embrittlement mechanisms that can work in various impurity-metal systems: drawing of charges from metal-metal bonds [47], difference between impurity segregation enthalpy at the grain boundary and the free surface [48], change of non-directional metallic bonds to more directional (less flexible) ones [49, 50] and, more recently, also an opposite transition from directional *s-d* bonds to more metallic (less strong) ones [11]. Using a combined theoretical (ab initio calculations) and experimental (electron energy loss spectroscopy) approach, the latter mechanism was proved to operate in the case of bismuth-induced embrittlement of copper grain boundaries [11, 51]. The copper atoms surrounding the segregated Bi exhibit a closed 3*d* shell, reduced *s-d* hybridization and an overfull *s* band. All these changes of electronic structure weaken the bonds between the copper atoms.

Hydrogen-induced embrittlement is believed to be caused by two basic mechanisms [52]: the hydrogen enhanced localized plasticity (HELP) and the hydrogen induced decohesion (HID). While HELP seems to predominantly underlie the intergranular fracture, HID was usually considered to be associated with the transgranular one. The latter consideration was supported by ab initio calculations of ideal fracture energy of Al {111} and Fe {110} surfaces as functions of hydrogen coverage θ [53]. These calculations revealed a steep linear decrease of both γ_{Al} and γ_{Fe} with increasing θ. However, more recent ab initio calculations [10] of binding energies of H with the grain boundary and the free surface in Ni indicate that, by virtue of the Rice-Wang theory [48], the HID mechanism can also work at grain boundaries. For bcc Fe, the predicted strong tendency to creation of both the linear hydrogen-vacancy complexes $VacH_2$-$VacH_2$ along the <111> direction and the planar clusters on {100} planes [10] deepens our understanding of both HELP and HID mechanisms in steels. Indeed, the vacancy rows along <111> slip direction may promote dislocation motions and the {100} clusters can lead to crack nucleation and cleavage on these planes.

Conclusion

Ab initio methods for calculation of uniaxial theoretical strength combined with stability analyses already give data that agree with experimental ones within a factor of two. This is already a plausible result owing to unavoidable imperfections of experimental tests. Values of both ideal shear strength and ideal binding energy are even more accurate and, therefore, they can be utilized as physical upper and lower bounds of shear strength and fracture toughness, respectively. Values of fracture energy of grain boundaries computed from first principles significantly help us to understand embrittlement mechanisms induced by hydrogen and impurity atoms. Thus, the superstructure of the bridge from interatomic bonds to local plasticity and fracture is quickly building and starts to carry a rising traffic on roads connecting these different scales.

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SOLUTION OF CRACK PROBLEMS BY THE OPTICAL METHOD OF CAUSTICS

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Summary. The limits of applicability and guidelines for the correct determination of stress intensity factors under opening-mode loading conditions by the optical method of caustics are presented. The use of optically anisotropic materials is introduced to obtain a double caustic which provides the state of stress, being plane strain, plane stress or three-dimensional, and therefore, the proper values of stress-optical constants for the correct determination of stress intensity factors.

INTRODUCTION

The optical method of caustics has extensively been used for the determination of stress intensity factors in crack problems (Gdoutos, 2005, Theocaris, Gdoutos, 1972). The method is based on the assumption that the state of stress near the crack tip is plane stress. However, experimental and analytical solutions have shown that the state of stress changes from plane strain near the crack tip to plane stress away from the tip through an intermediate region where the stress state is three-dimensional (Konsta-Gdoutos, Gdoutos, 1992). The changing state of stress results to changing values of stress-optical constants which enter in the equations for the determination of stress intensity factors. For the correct determination of stress intensity factors the proper values of stress-optical constants should be used.

THE OPTICAL METHOD OF CAUSTICS

In the optical method of caustics a specimen is illuminated by a light beam and the reflected or transmitted rays from the front or rear face of the specimen undergo a change of their optical path, due to the variation of the thickness and/or the refractive index dictated by the stress field (Fig. 1). At stress gradients resulting at crack tips, the reflected or transmitted rays generate a highly illuminated three-dimensional surface in space. When this surface is intersected by a reference screen, a bright curve, the so-called caustic curve, is formed. For transparent materials three caustics are formed by the light rays reflected from the front and rear surfaces and those transmitted through the specimen. For opaque materials, only one caustic is formed by the reflected light rays from the front surface of the specimen. The dimensions of the caustic are related to the state of stress near the crack tip. For the case of a mode-I through-the-thickness crack the stress intensity factor K_{exp} is given by

$$K_{exp} = 0.0934 \frac{D^{5/2}}{z_0 \, c \, t \, m^{3/2}} \qquad (1)$$

where z_0 is the distance between the specimen and the viewing screen where the caustic is formed, c is the stress optical constant of the specimen under conditions of plane stress, t is the specimen thickness, m is the magnification factor of the optical arrangement defined as the ratio of a length on the reference screen where the caustic is formed divided by the corresponding length on the specimen and D is the transverse diameter of the caustic at the crack tip. The above equation is valid when the state of stress in the vicinity of the crack tip is plane stress, so that the value of stress-optical constant under conditions of plane stress is used.

For optically isotropic materials, the caustic is created by the light rays reflected from the circumference of a circle, the so-called initial curve, which surrounds the crack tip. The radius of the initial curve is given by

$$r = 0.316 D \qquad (2)$$

EXPERIMENTAL RESULTS

Experiments have shown that the stress intensity factors determined by caustics corresponding to various values of the radius of the initial curve vary with the distance from the crack tip and reach a plateau value for distances from the tip approximately greater than half the specimen thickness. In these experiments the value of the stress-optical constant entering in the determination of stress intensity factor was obtained equal to the plane stress value. Conditions of plane stress dominate at distances from the tip greater than half the specimen thickness. For distances smaller than half the specimen thickness, where the state of stress is plane strain or three-dimensional the appropriate value of stress-optical constant should be used.

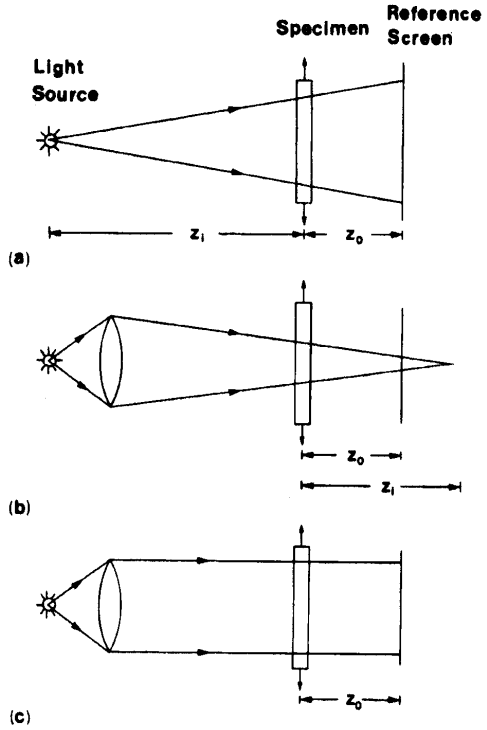

Fig. 1 Optical arrangement for divergent (a), convergent (b) and parallel (c) light

Fig. 2 presents the variation of K_{exp}/K_{th} versus r/d for a value of the specimen thickness d = 4.5, and different values of specimen width. Points in figure correspond to different values of the applied load, P, the magnification factor of the optical arrangement, m, the distance between the specimen and the viewing screen where the caustic is formed, z_0, and the specimen thickness, d. Note form figure that the ratio K_{exp}/K_{th} increases with r/d and reaches a plateau value equal to one as the radius of the initial curve takes a limiting value r_c. At that value of $r = r_c$ the state of stress in the neighborhood of the crack tip becomes plane stress. For distances r smaller than r_c the state of stress is three-dimensional, while for values of r larger than r_c plane stress conditions dominate. It was obtained that the critical value of r for which the state of stress becomes plane stress depends not only on d, but also on the geometrical characteristics of the cracked plate, especially the ratio of the crack length to specimen thickness.

LIMITS OF APPLICABILITY OF THE METHOD OF CAUSTICS

The condition that the initial curve of the caustic should lie at distances from the tip approximately greater than half the specimen thickness introduces limitations in the parameters (distance between the specimen and the viewing screen where the caustics is formed, the magnification factor of the optical arrangement, the specimen dimensions and thickness, and applied loads) entering in the determination of stress intensity factors. These factors should be properly selected so that the initial curve lies in the region where plane stress conditions dominate. In that case the value of stress-optical constant corresponding to plane stress should to be used.

In order to obtain caustics generated from the region of plane stress the radius of the initial curve of the caustic should be larger than a fraction of the specimen thickness. By taking this distance equal to half the specimen thickness we obtain

$$\left(\frac{3.385 z_0 c K}{m}\right)^{2/3} > d \qquad (3)$$

Inequality (3) establishes a condition the quantities, z_0, c, K, m, d should satisfy in order to obtain caustics generated by an initial curve that lies in the plane stress region Fig. 3 presents the variation of the critical (maximum) value of specimen thickness, d_c, versus K_I for z_i = 0.8 m for a divergent light beam illuminating a notched Plexiglas specimen. z_i represents the distance between the point light source and the specimen. Observe that the critical thickness d_c increases as K_I, z_0, z_i increase.

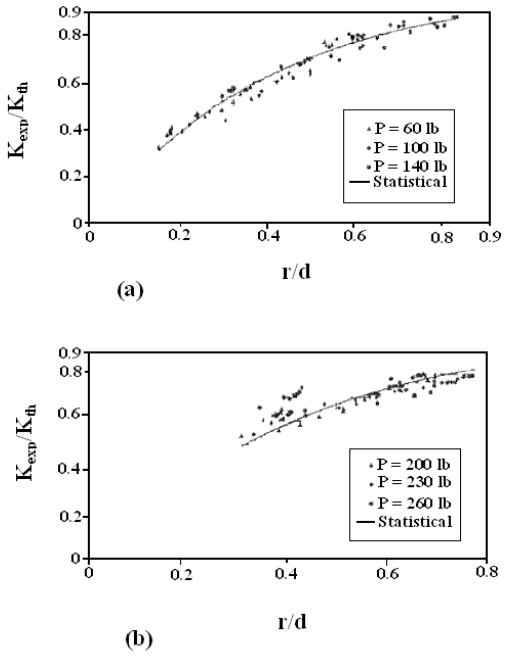

Fig. 2 Variation of K_{exp}/K_{th} versus r/d for a = 15.5 mm, d = 4.5 mm and w = 47.5 mm (a) and w = 63.5 mm (b)

DETERMINATION OF STRESS INTENSITY FACTORS

When the initial curve of the caustic lies at distances where three-dimensional effects dominate the proper value of the stress-optical

constant, c, should be used. The value of the stress-optical constant changes from its plane strain value near the tip to its plane stress value at distances away from the tip approximately equal to half the specimen thickness. In order to characterize the three-dimensionality of the stress field near the crack tip an empirical triaxiality factor k is introduced, such that

$$\sigma_z = k\nu\left(\sigma_x + \sigma_y\right) \qquad (4)$$

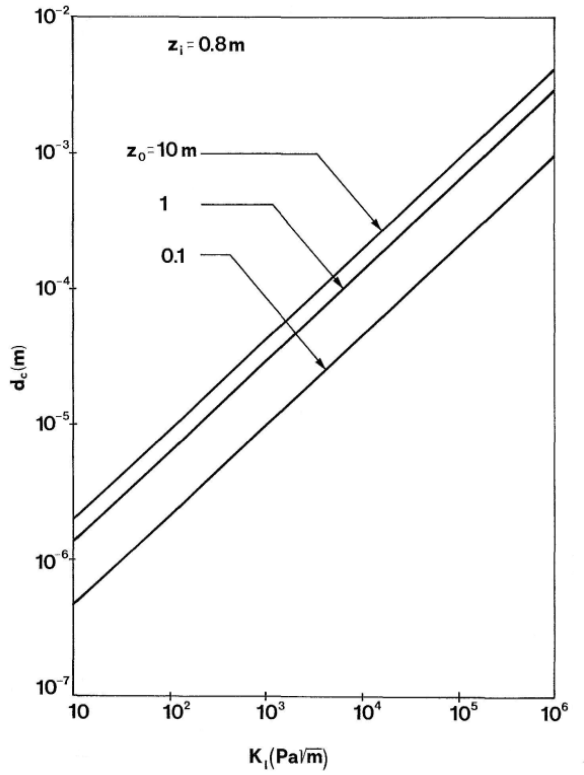

Fig. 3 Variation of maximum value of d (d_c) versus K_I for divergent light. z_i= 0.8 m, and z_0 = 0.1, 1 and 10 m.

where σ_z is the normal stress perpendicular to the plane of the specimen, and σ_x and σ_y are the in-plane stresses. k takes the values of 0 and 1 for plane stress ($\sigma_z = 0$) and plane strain [$\sigma_z = k\nu\left(\sigma_x + \sigma_y\right)$], respectively.

When the triaxiality factor is determined the corresponding value of the stress-optical constant, c, is calculated which subsequently is used for the determination of stress intensity factor. Fig. 4 presents the variation of the stress-optical constant c_t for transmitted light for Plexiglas (PMMA) versus the triaxiality coefficient k from its plane stress (k = 0) to its plane strain value (k = 1) for various values of the index of refraction n_0 of the surrounding medium. Note that c_t varies linearly with k. From Fig. 4 it is observed that c_t remains almost constant for n_0 = 1.3. This means that when the index of refraction of the medium surrounding the specimen is equal to n_0 = 1.3 the stress-optical constant c_t is independent of the state of stress near the crack tip. Under such circumstances Eq. (1) can be used for the correct determination of stress intensity factor K_I for any values of the parameters entering in Eq. (1).

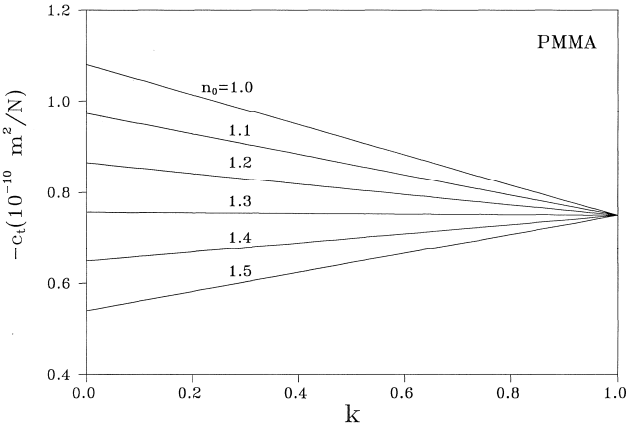

Fig. 4 Variation of stress-optical constant c_t versus triaxiality coefficient k for PMMA for various values of the index of refraction n_0 of the surrounding medium. k = 0 and 1 correspond to conditions of plane stress and plane strain, respectively.

USE OF OPTICALLY ANISOTROPIC MATERIALS

In optically anisotropic materials the variation of the optical path of a light ray traversing the specimen along the two principal stress directions is given by (Theocaris and Papadopoulos, 1981):

$$\Delta s_{t1,2} = c_t\left[\left(\sigma_1 + \sigma_2\right) \pm \xi_{r,t}\left(\sigma_1 - \sigma_2\right)\right]d \qquad (5)$$

where the coefficient $\xi_{r,t}$ characterizes the optical anisotropy of the material for light rays reflected from the rear face or traversing the specimen. The plus and minus signs in equation correspond to the values σ_1 and σ_2 of the principal stresses. Under such conditions the parametric equations of the caustic are given by:

$$X_{r,t} = \left(\frac{3}{2}c_{r,t}\right)^{2/5}\left[A^{2/5}\cos\theta + \frac{2}{3}A^{-3/5} x\left\{\cos 3\theta/2 \pm \frac{3}{4}\xi_{r,t}\sin 2\theta\right\}\right] \qquad (6a)$$

$$Y_{r,t} = \left(\frac{3}{2}c_{r,t}\right)^{2/5}\left[A^{2/5}\sin\theta + \frac{2}{3}A^{-3/5} x\left\{\sin 3\theta/2 \pm \frac{1}{4}\xi_{r,t}\left(1+3\cos 2\theta\right)\right\}\right] \quad (6b)$$

where:

$$A = \pm\xi_{r,t}\sin\theta + \left[1 \pm \xi_{r,t}\left(7\sin\theta/2 - \sin 3\theta/2\right) + \frac{1}{32}\xi_{r,t}^2\left(25+9\cos 2\theta\right)\right] \quad (7)$$

$$C_{r,t} = \frac{\varepsilon z_0 d c_{r,t} K_1}{(2\pi)^{1/2}}$$

The equation of the initial curve is given by:

$$r = r_0 = \left\{\frac{3}{2}C_{r,t}A\right\}^{2/5} \quad (8)$$

Equations (6) express the equations of the caustic curve for optically anisotropic materials. Two caustics are obtained corresponding to the plus and minus signs in equations. These caustics are referred to the two principal stress directions. Note that for $\xi_{r,t} = 0$ equations (6) and (8) reduce to the equations of the caustic for optically isotropic materials [2]. Fig. 5 shows the initial curves and respective caustics in a plate with crack subjected to tension made of birefringent materials with ξ = 0, 0.2, 0.4, 0.6, 0.8 and 1.0. Observe that as ξ increases the shapes of the initial curves and caustics are progressively distorted. The distance between the two caustics increases as ξ also increases. The value of ξ depends on the state of stress, being plane strain, plane stress or three-dimensional. Thus the experimental caustics obtained can be used for the determination of the triaxiality factor *k* and the subsequent calculation of the stress-optical constant for the correct determination of stress intensity factors.

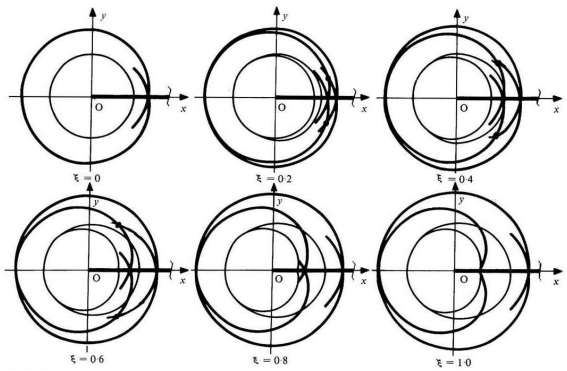

Fig. 5 Initial curves and respective caustics in a plate with crack subjected to tension made of birefringent materials with ξ = 0, 0.2, 0.4, 0.6, 0.8 and 1.0

CONCLUSIONS

From the results of the present work the following conclusions may be drawn:

a. Direct application of the method of caustics without taking special precautions for the determination of stress intensity factors may lead to erroneous results.

b. The material, dimensions of the specimen, applied loads and geometrical dimensions of the optical arrangement should be properly selected to ensure that the initial curve lies in the plane stress region.

c. The above condition is satisfied for high applied loads, small specimen thicknesses, large distances between the specimen and the viewing screen and small magnification factors of the optical arrangement.

d. For specimens made of Plexiglas the stress-optical constant for transmitted light rays is independent of the state of stress around the crack tip for a value of the index of refraction of the medium surrounding the specimen approximately equal to 1.35. Under such condition the plane stress stress-optical constant of the material can be used for any location of the initial curve of the caustic.

e. Optically anisotropic materials can effectively be used for the determination of the state of stress around the initial curve of the caustic and the correct determination of stress intensity factors. For such materials the two caustics formed can be used for the determination of the triaxiality coefficient and the subsequent calculation of the corresponding stress-optical constant.

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