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2nd International Workshop on Physics-Based Modelling of Material Properties and Experimental Observations with special focus on Fracture and Damage Mechanics

Book of abstracts

Karl-Fredrik Nilsson, Tunçay Yalçinkaya,
Ersin Emre Oren, Cihan Tekoğlu

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2nd International Workshop on Physics-Based Modelling of Material Properties and Experimental Observations with special focus on Fracture and Damage Mechanics

Book of Abstracts

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Introduction

The Workshop is funded by the EU Enlargement & Integration Action (E&IA) and, co-organized by the Institute of Energy and Transport and the Joint Research Centre (JRC) and TOBB University of Economics and Technology (TOBB ETU), .The objective of the workshop is to discuss the present status of physics-based models to predict material degradation and failure of mechanical components. Such approaches allow a better understanding of how the material microstructure, environment and loadings affect degradation and failure mechanisms. This is important for the design of new materials with tailored damage resistant properties as well as for more accurate predictions of safety margins and failure probabilities of components of specific materials. Physics-based models are also necessary for extrapolation of data beyond operational experience and for correctly predicting the transferability between specimen tests and real components.

The structural integrity and functioning of mechanical components is affected by initial defects as well as by time dependent degradation mechanisms such as creep, fatigue, stress corrosion cracking, irradiation embrittlement and thermal ageing. The modelling and understanding of degradation mechanisms and the predictability of failure loads is constantly evolving. Recently, we have seen a trend towards physics-based models that simulate the degradation and failure processes and mechanisms that operate at different length and time scales. Such approaches allow us to make better prediction of long-term performance and safety margins, transferability between specimens and components.

The Workshop consists of nine Keynote lectures from renowned international experts, covering different areas related to physics-based models for damage and fracture; 18 oral presentations and more than 20 Poster presentations. The workshop presentations give an overview of different physics-based models for fracture and degradation of primarily metallic materials and how they can be used for improved understanding and more reliable predictions. Models addressed include cohesive zone models to simulate fracture processes, ductile-brittle transition for ferritic steels, ductile fracture mechanisms such as void growth or localized shear, fatigue crack initiation and short crack growth and assessment of protective coatings. Experimental studies that support such models and case studies that illustrate their use are also within the scope. The Workshop gives an opportunity for scientists and engineers from EU Member States and target countries to discuss research activities that could be a basis for future collaborations.

Technical Program

WEDNESDAY, MAY 15

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09:00 – 09:20 Opening: Hatice Duran (TOBB-ETÜ) and Karl-Fredrik Nilsson (EC-JRC)

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09:40 – 11:00 Key Note Lectures *(Session I)*

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10:20 – 11:00 Nonequilibrium thermodynamics of surfaces and interfaces in solids with applications, T.O. Ogurtanı, Middle East Technical University, Turkey

11:00 – 11:30 Coffee Break

11:30 – 12:30 Oral Presentations *(Session I)*

11:30 – 11:50 Towards development of hydrogen embrittlement resistant steel alloys, T.M. Hatem, British University in Egypt

11:50 – 12:10 A fracture criterion for the notch strength of high strength steels in the presence of Hydrogen, C. Ayas, Cambridge University, UK

12:10 – 12:30 Overview of peridynamic theory: past and present, E. Oterkus, University of Strathclyde, UK

12:30- 14:00 Lunch

14:00 – 15:20 Key Note Lectures *(Session II)*

14:00 – 14:40 Comparison between pile-up singularities and stress fields induced by slip bands. Application to the prediction of grain boundary microcrack nucleation, Maxime Sauzay, CEA, France

14:40 – 15:20 Recent Advances in Phase Field Modeling of Brittle and Ductile Fracture, C. Miehe, University of Stuttgart, Germany

15:20 – 15:50 Coffee Break

15:50 – 17:10 Oral Presentations *(Session II)*

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16:10 – 16:30 Influence of hydrogen on dual phase steel deformation micro-mechanics, C.C. Tasan, Max-Planck-Institut für Eisenforschung, Germany

16:30 – 16:50 The scale transition procedure for constitutive equations in multilevel models based on crystal plasticity, Alexey I. Shveykin, Perm National Research Polytechnic University, Russia

16:50 – 17:10 XFEM applications for integrity analysis of Reactor Pressure Vessels cracked walls, V. F. González Albuixech, PSI, Switzerland

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09:40 – 10:20 Applications of advanced micromechanics based ductile failure models - Do we really need all this complexity?, T. Pardoen, Université catholique de Louvain, Belgium

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11:10 – 11:30 Strain-induced damage of metals under large plastic deformations, M. Zapara, Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

11:30 – 11:50 Comparing two models for slip-patterning and strain-localization based on a non-convex plastic energy, G. Lancioni, Università Politecnica delle Marche, Italy

11:50 – 12:10 Ductile damage model for metal forming simulations including physics based modeling of void nucleation, A.V. Shutov, Chemnitz University of Technology, Germany

12:10 – 13:40 Lunch

13:40 – 14:20 Key Note Lectures (Session IV)

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14:40 – 15:40 Oral Presentations (Session IV)

14:40 – 15:00 Transferability of brittle fracture properties for different specimens and prediction of fracture toughness for RPV steels, V. Kostylev, Prometey, Russia

15:00 – 15:20 The prestrain effect on brittle fracture: physical features, mechanical modeling and application for RPV steels, V. Shvetsova, Prometey, Russia

15:20 – 15:40 Crack-like defects in welded joints - heterogeneity and constraint effects on fracture behaviour, A. Sedmak, Univ. of Belgrade, Serbia

15:40 - 17:40 Poster Session

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09:40 – 10:20 Ductile failure at low stress triaxiality, J. Faleskog, Royal Institute of Technology, Sweden

10:20 – 10:40 Coffee Break

10:40 – 12:00 Oral Presentations (Session V)

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11:00 – 11:20 Structure residual life assessment with fatigue process specific accounting, S. Yutskevych, National Aviation University, Ukraine

11:20 – 11:40 Viscoelasticity and high buckling stress of dense carbon nanotube brushes, G. Cambaz-Büke, Cankaya University, Turkey

11:40 – 12:00 Experimental and computational investigation of dynamic crack growth along curved interfaces, D. Çöker, Middle East Technical University, Turkey

12:00 – 12:30 Closing of Workshop

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Poster 2	*Structural reliability approach in thermal fatigue crack growth by stochastic modeling* V.S. Radu Institute for Nuclear Research, Arges, Romania
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Poster 7	*A three dimensional model for nanocrystalline materials based on grain interior and grain boundary deformation mechanisms* E. Gürses Department of Aerospace Engineering, Middle East Technical University (METU), Ankara, Turkey
Poster 8	*Crystal plasticity based prediction of creep and microcracking in irradiated polycrystalline graphite* L. Delannay[1], J.F.B. Payne[2], N. Tzelepi[2] [1] Université Catholique de Louvain (UCL), iMMC-MEMA, av. G. Lemaître, 4 – B1348, Louvain la Neuve – Belgium; [2] National Nuclear Laboratory (NNL), Stonehouse Park, Bristol road, Stonehouse, GL10 3UT, United Kingdom
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Opening and Keynote speakers

The need for physics-based fracture and damage models for nuclear energy applications

Karl-Fredrik Nilsson and Tuncay Yalçinkaya

Institute for Energy and Transport, Joint Research Centre, European Commission
PO Box 2, 1755ZG, Petten, The Netherlands

Nuclear energy is one of the fields which could benefit most from physics-based models for fracture, damage and degradation. This need is driven by:

- the very high safety requirements for nuclear components;
- the extreme environment that nuclear components are exposed to with respect to irradiation damage, high temperatures and environmental degradation effects from the coolants;
- long-term effects exemplified by at least 60 years design-life for future reactors and life-extension of present reactors to 60 or even 80 years.

The presentation will give some snap-shots of where advanced physics-based models could provide more accurate predictions or better understanding.

One parameter fracture models (J or K) do not capture the effects of loading and geometry and should normally provide conservative estimates. Hence there is a transferability issue between using the parameters determined from specimen tests and application to components. More accurate predictions may be needed to demonstrate safety margins. This can be achieved by a two-parameter approach (e.g. J-Q) where the second parameter is a measure of the stress triaxiality. Further improvements can be achieved by models that simulate the fracture process such as cohesive zone models or void growth and coalescence models.

Irradiation damage is the most specific nuclear specific degradation mechanism. The neutron irradiation induces point defects and nuclear transmutation of elements resulting in reduced ductility and fracture toughness at the component scale. Modelling of irradiation damage is a multi-scale problem that covers the whole range of time and size scales from atomistic via meso-scale to the component scale where the macro properties are of interest. Models include molecular dynamics, dislocation dynamics, crystal plasticity as well continuum mechanics.

The operational conditions and end-of-life material properties can often not be simulated directly by experiments. One approach to mitigate long-term degradation mechanisms is to have a surveillance programme where some specimens are located where the harshest conditions prevail. The degradation and associated material properties of these components can then be monitored. Physics-based models can then be an essential tool in understanding the basic mechanisms and provide an important tool in the safety assessment. At the laboratory scale one must rely on some kind of accelerated tests from which we need to extrapolate or interpolate to predict the end-of-life properties. Examples are creep-tests accelerated by higher load or temperatures and irradiation tests where special fast neutron facilities would be required to get sufficient irradiation damage levels. Such an approach requires that we can model the key degradation mechanisms and that they remain the same, or at least that we can predict the change.

Thus it is clear that physics-based model development need to be seamlessly integrated with experimental work..

Fracture Mechanics of Coatings

John W. Hutchinson

School of Engineering and Applied Sciences, Harvard University

Coatings on substrates fail in numerous ways. Coatings under tension can experience through-cracks which, once triggered, can propagate across the entire coating and which generally increase in density as the tension increases. Coatings in tension can also experience delamination within the coating or substrate or at the coating-substrate interface, depending on the relative toughness of the coating, substrate and interface. Coatings in compression can experience either edge delamination or buckle delamination. The mechanics of this rich array of failure modes will be briefly reviewed and discussed within the context current technological applications. To illustrate efforts underway to improve coatings, one of the most important thermal barrier systems for turbine engine blades will be discussed which delaminates at the interface between the thermally grown oxide, alumina, and the metal bond coat which bonds the ceramic thermal barrier to the superalloy blade. In service, this interface accumulates contaminates which can reduce the intrinsic atomistic separation energy and it loses its planarity by undulations that develop under the cyclic thermal history imposed on the blade. Thus, both the intrinsic toughness of the interface and the local mechanical stresses it experiences change with time. This example will be used to motivate issues related to understanding and modeling the mechanics of interface fracture. To date, robust methods for the lifetime assessment of thermal barrier coatings have not emerged based on models of the degradation processes due to their complexity. In the absence of mechanism-based predictive models of toughness degradation, direct measurement of coating adherence as a function of thermal exposure must be a component of any practical approach toward lifetime assessment. The presentation concludes with an outline of an approach to lifetime assessment of TBC that has taken shape in the past few years, including ways for dealing with one of the most serious environmental problems—dust ingestion in the engine which melts when it strikes the turbine blades and penetrates the ceramic coatings.

Simulation of Crack Extension by Cohesive Elements

Wolfgang Brocks

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As R-curves based on classical parameters of fracture mechanics like J suffer from geometry dependence and have limited predictive capabilities, new concepts like CTOA-controlled crack extension, cohesive models and continuum damage mechanics emerged and find increasing interest, all necessitating computational tools. Cohesive elements have in particular proven their ability in modelling crack extension in thin-walled panels and shells, and their respective parameters provide physically meaningful measures of the materials fracture toughness and tearing resistance.

The concept is attributed to Barenblatt (1959) who introduced a cohesive zone in the ligament of the crack, where material degradation occurs and stresses remain finite. His model became more interesting for practical applications when numerical methods, in particular the FEM, were applicable to nonlinear problems. The material separation und thus damage of the structure is described by interface elements, obeying some decohesion law, whereas the continuum elements around remain damage-free. When damage occurs, the interface elements open according to some law of decohesion and finally lose their stiffness at failure so that the continuum elements are disconnected.

The concept of a cohesive interface at the boundary of adjacent continuum elements that allows for material separation is a useful, versatile and well-established tool for many kinds of fracture mechanisms. The cohesive zone is a phenomenological model but based upon a sound physical background. Cohesive models can be applied to problems with or without initial cracks, i.e. classical fracture mechanics as well as debonding problems. As they represent a local approach, they are less sensitive to any geometry dependence of their parameters.

The model can be applied on various lengthscales from the structural (macro) to the material (micro) scale. It is also capable of predicting crack branching and bifurcation. A suitable meshing is crucial to realise the actual crack path, however.

An overview of the state of the art is given, see e.g. Brocks et al. (2003), and a number of examples is presented to illustrate the manifold applications. Problems of parameter identification and transferability are discussed.

Barenblatt, G.I. (1959): The formation of equilibrium cracks during brittle fracture: general ideas and hypothesis, axially symmetric cracks. Appl. Math. Mech. 23, 623-636.

Brocks, W.; Cornec, A.; Scheider, I. (2003): Computational aspects of nonlinear fracture mechanics. In: Comprehensive Structural Integrity - Numerical and Computational Methods, Milne I, Ritchie RO, Karihaloo B.(eds), Vol. 3, Elsevier 2003; 127-209.

Ductile Failure at Low Stress Triaxiality

Jonas Faleskog

Department of Solid Mechanics, Royal Institute of Technology, Stockholm, Sweden

Ductile failure in metal alloys is, in one way or another, attributed to nucleation, growth and coalescence of voids. This failure process is fairly well understood under high stress triaxiality, but less so for stress states at low triaxiality. However, recent micromechanical studies show that under shear dominated stress states, void driven ductile failure may even occur when triaxiality becomes negative, but with a very different behaviour. Under such circumstances voids deforms into penny shaped cracks that rotate and start to interact in a manner that leads to coalescence and material failure. This behaviour has also been observed experimentally, and continuum damage models have started to emerge addressing this phenomenon.

Another interesting trend brought out from these experiments is that in some metallic alloys, the critical effective plastic strain is not monotonically related to triaxiality. The distinction between axisymmetric stress states and shearing stress states becomes important when assessing ductility in these alloys, as they have less ductility in pure shear than under axisymmetric states with markedly higher triaxiality. The distinction between axisymmetric and shearing stress states can be expressed by use of the third deviatoric stress invariant J3. Moreover, experimental results seem to suggest that in metallic alloys where the plastic flow properties (yield criterion etc.) does depend on J3 in a marked way, the distinction between axisymmetric and shearing stress states is less important for ductility. This will to some extent be illustrated by results from an analysis based upon a Gurson type of model extended to account for J3 in the plastic flow properties of the matrix material.

To summarize, in this presentation, recent experiments on ductile failure in the low triaxiality regime will be reviewed, micromechanical void studies illustrating low triaxiality failure will be discussed and results from analysis based on recently proposed continuum damage constitutive models will be used to demonstrate their capability to capture essential aspects observed in experiments.

Micromechanically-based Models of Ductile Fracture

Jean-Baptiste Leblond

Institut Jean Le Rond d'Alembert, Université Pierre et Marie Curie, Paris France

This talk will provide an introduction to classical constitutive models for plastic porous materials based on micromechanical analyses of the elementary mechanisms of ductile rupture, and review a few recent directions of research in this area. It will encompass five topics:

1) A presentation of Gurson's classical model for voids of spherical shape, based on some approximate limit-analysis of a hollow sphere subjected to conditions of homogeneous boundary strain rate.

2) The commonly observed acceleration of ductile rupture arising from cyclic loadings; the physical origin of the phenomenon will be explained and its incorporation into some constitutive model will be discussed.

3) A presentation of a very recent model of ductile fracture accounting for void shape effects, standing as an extension of Gurson's model for spherical voids to voids of arbitrary ellipsoidal geometry.

4) The extension of Thomason's classical work on coalescence of voids subjected to simple tension with superimposed hydrostatic tension, to fully general loadings including shear components.

5) The issue of unlimited localization of strain and damage in standard first-gradient models, and a possible solution to this problem in the form of some second-gradient model obtained by extending Gurson's limit-analysis to conditions of inhomogeneous boundary strain rate.

Multi-scale brittle fracture modeling and prediction of fracture toughness for irradiated RPV steels

Boris Margolin

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The main objectives of the present lecture are (i) to analyse applicability of available local cleavage fracture criteria for radiation embrittlement modelling; (ii) to develop models of the effect of radiation-induced defects on the processes of cleavage microcrack nucleation and propagation; (iii) to consider application of brittle fracture models for prediction of fracture on a macro-scale for irradiated RPV materials.

Two local criteria that are currently widely used for brittle fracture prediction are considered from viewpoint of radiation embrittlement modelling: stress-controlled criterion used in the RKR and Beremin models, and stress-and-strain controlled criterion used in the Prometey model. The stress-controlled criterion that is actually based on cleavage microcrack propagation condition, describes radiation embrittlement as a result of material hardening only. Brittle fracture according to the stress-and-strain controlled criterion may be controlled both by cleavage microcrack propagation and nucleation.

It has been found that radiation embrittlement is not only due to the hardening of material as traditionally considered. Damage features such as irradiation-induced lattice defects, element precipitation and impurity segregation also affect cleavage microcrack nucleation, although they do not appreciably change the critical stress for microcrack propagation. It is shown that radiation embrittlement of RPV steels is connected both with the increase of yield stress (mechanical factor) and the decrease of the critical stress for microcrack nucleation (physical factor). Physical-and-mechanical models of the effect of radiation defects on cleavage microcrack nucleation are proposed. The dependence of critical stress for microcrack nucleation on neutron fluence is obtained allowing for various radiation-induced defects. On the basis of the obtained results an appearance of the mode of intergranular fracture for RPV steels after irradiation and post-irradiation annealing is analysed and explained.

The Prometey model is applied for fracture toughness prediction for irradiated RPV materials. It has been shown that the Prometey model provides not only a prediction of the KJC(T) curve allowing for possible variation in the KJC(T) curve shape but, at present, is the only model that allows the prediction of lateral shift of KJC(T) curves.

On the basis of the Prometey model an engineering method named the Unified Curve method has been developed for prediction of KJC(T) curve. The Unified Curve method is simple as the Master Curve method but in contrast to the latter the Unified Curve method takes into account a variation in the KJC(T) curve shape when a degree of material embrittlement increases. The Master Curve is a partial case of the Unified Curve.

The Prometey model is also applied for modeling the effect of material hardening caused by cold work on brittle fracture. As known, material hardening due to cold work may result in both decreasing and increasing fracture toughness (as distinct from the hardening caused by irradiation always resulting in material embrittlement). It has been shown that these findings may be explained only with the developed model.

Applications of advanced micromechanics based ductile failure models
Do we really need all this complexity ?

T. Pardoen

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The most advanced versions of Gurson type models available today combine:

(i) a composite homogenization theory based void nucleation law involving distribution of nucleation strength;

(ii) an enhanced description of void growth involving void shape and rotation, viscoplasticity, kinematic hardening and plastic anisotropy;

(iii) a model for the onset of void coalescence rooted on micromechanics taking into account effects of shear and second population of voids;

(iv) a physics based model for the final unloading of a material element undergoing coalescence.

Contrarily to the often conveyed idea, the number of parameters involved in this class of models remains limited while being well defined by the microstructure and by classical plastic flow properties. Nevertheless, only a few elements of the complex multifold model described above are generally needed to address real applications, tough varying from one application to another.

Educated choices of the right assumptions heavily rely on in depth analysis of properly selected experiments. Several applications dealing with fracture of Al alloys will be reviewed to reveal the kind of decisions that have to be taken and the importance of several of the model enhancements worked out in recent years. The process will be illustrated by following examples all related to industrial applications:

- fracture of 6xxx Al series alloys for extrusion,
- 6xxx Al friction stir welded joints of thin Al sheets,
- 7xxx series Al alloys with precipitate free zones,
- cast Al alloys and strain hardening effects for Al fracture toughness.

Comparison between pile-up singularities and stress fields induced by slip bands. Application to the prediction of grain boundary microcrack nucleation

Maxime Sauzay

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Slip localization is widely observed in metallic polycrystals, for instance after tensile deformation, cyclic deformation (persistent slip bands) or pre-irradiation followed by tensile deformation (channels). Such strong deformation localized in thin slip bands induces local stress concentrations in the quasi-elastic matrix around, at the intersections between slip bands and grain boundaries (GBs) where microcracks have been often observed.

Since the fifties, such stress fields have been modeled using the dislocation pile-up theory which leads to stress singularities similar to the LEFM ones. Following the pioneering works of Zener, Mott and Stroh, the Griffith criterion has then been widely applied because of the stress singularity exponent, 1/2. But this usually leads to strong underestimations of the remote stress to GB microcrack initiation. In fact, slip band thickness is finite: 50nm-1000nm depending on material, temperature and loading conditions. Therefore, many slip planes are plastically activated through the thickness. To evaluate more accurately the local stress fields, crystalline finite element (FE) computations are carried out using microstructure inputs such as slip band aspect ratio and spacing. Slip bands of low critical resolved shear stress (CRSS) are embedded in a matrix or small aggregates (high CRSS) (Fig. 1 a, zoom).

General formulae inspired by the theory of matching expansions are deduced from the FE results. The normal and shear stress fields in the vicinity of the slip band are much lower than predicted by the pile-up theory (Fig. 1 b).

Then the J-integral is computed depending on the intergranular crack length. This finally allows us to apply finite fracture mechanics and a double fracture criterion using both critical stress and fracture energy. The GB microcrack initiation predictions are in much better agreement with the experimental observations than the pile-up ones.

Finally the influence of the random features of polycrystalline microstructure is studied in details (crystal orientation, GB plane, neighbor grains, parallel slip bands…), which may explain the random and continuous GB crack initiation at the surface of polycrystals.

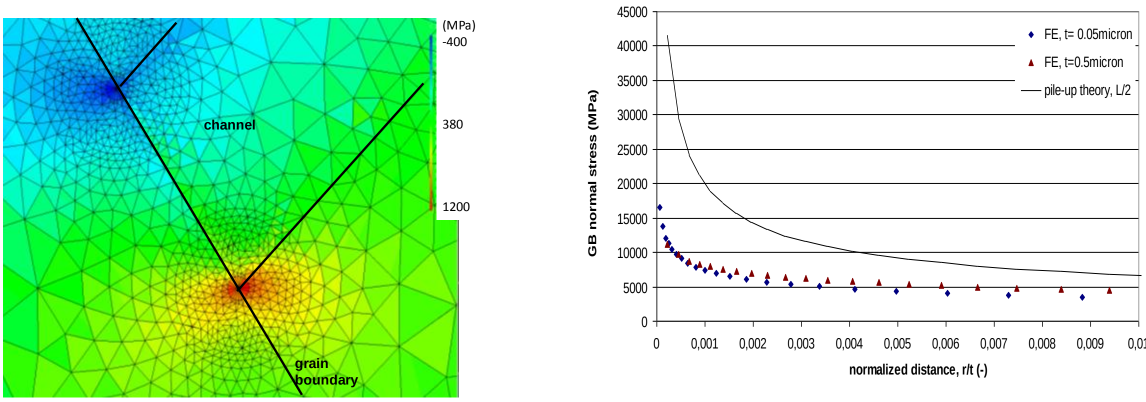

Figure 1 : a) axial stress field in the vicinity of the slip band – GB intersection (remote tensile stress : 300MPa ; b) comparaison between GB normal stress fields computed by the FE method (finite thickness, t) or by the pile-up theory (remote stress: 700MPa, grain size: 10 μm*).*

Nonequilibrium Thermodynamics of Surfaces and Interfaces in Solids with Applications

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The realization of nanoscale devices largely depends on our ability to control and manipulate interfacial interactions and thus understanding the mechanisms of surface/interface instabilities. The morphological changes and instabilities of strained solid surfaces and interfaces under various environmental conditions continue to be challenging theoretical/technological problems. By drawing from elegant fundamental laws of physics and chemistry, the field allows for the exciting possibility of making quantitative prediction about the behavior of a diverse range of real materials. Wetting, sintering, grain growth, grain boundary grooving, growth of thin films, and stability of multilayers are all examples of capillary driven shape and microstructural evolution.

Hitherto, all theoretical studies related to the interfaces and surfaces rely strictly on the use of classical thermodynamics as a general tool for the macroscopic description of physico-chemical processes. Additionally some obscure modifications in the concept and usage of chemical potentials and the free energies have been included especially in the presence of externally imposed force fields, without considering their definitions. More serious limitations lie in the fact that the methods are based on reversible processes and true equilibrium states.

In this work, we present the formulation of two distinct thermodynamic systems (isobaric/isochoric) by using irreversible thermodynamics in conjunction with the generalized variational method. The result is a well-posed moving boundary value problem describing the dynamics of curved interfaces and surfaces associated with voids and/or cracks that are intersected by grain boundaries. To do this, we followed the Fowler/Guggenheim interpretation of the Planck inequality for isothermal, natural and reversible infinitesimal changes in heterogeneous systems. Combining this basic principle with the interlink between the dissipation function and the global internal entropy production provided us two diverse sets of governing equations for the surface drift-diffusion flux plus the rate of evaporation/condensation. This study shows that the role of the energy-momentum tensor in the generalized potential for the interface displacement is different (opposite in sign) for isochoric and isobaric systems. That means, on the contrary to the common belief, the elastic strain energy density contributes to the generalized driving force for the surface drift-diffusion alone by favoring flat and smooth surfaces in isobaric systems (healing), rather than causing the surface roughness and even crack initiation as in internally strained isochoric systems.

Based on the theory developed, extensive computer simulations are performed for void configuration evolution during intergranular motion, grain grooving and the evolution behavior of epitaxial thin films and quantum dots formations. *Supported by TUBITAK grant no 111T343*.

Recent Advances in Phase Field Modeling of Brittle and Ductile Fracture

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The computational modeling of failure mechanisms in solids due to fracture based on sharp crack discontinuities suffers in dynamic problems with complex crack topologies including branching. This can be overcome by a diffusive crack modeling based on the introduction of a crack phase field as proposed in [1-4]. Recently, we extended these models of brittle crack propagation towards the analysis of ductile fracture in inelastic solids undergoing finite strains, including thermo– and chemo–mechanical coupling scenarios. In particular, we propose a formulation that is able to predict brittle-to-ductile failure mode tansitions in metals and polymers under dynamic loading at finite elastic–plastic strains. The proposed model is able to reproduce classical impact tests of metal specimes, which show brittle-toductile failure mode transition for increasing impact velocity. Similar failure mode transitions occur in glassy polymers due to the competition of shear yielding and crazing.

A thermodynamically consistent framework is outlined for continuum phase field models of crack propagation in brittle elastic and ductile elastic-plastic solids, including its robust numerical implementations by multi-field finite element methods. The investigation starts with an intuitive and descriptive derivation of a regularized crack surface density function. This function provides the basis for the construction of suitable dissipation functions, which govern the degrading stress response in ductile materials, the evolution of plastic strains and temperature as well as the crack phase field.

Local history fields are introduced which contain suitably defined crack driving forces related to alternative failure criteria. It is shown that these local variables drive the evolution of the crack phase field. The introduction of the history fields inspires the construction of extremely robust operator split schemes of phase-field-type fracture which successively update in a typical time step the history fields, the crack phase field and finally the deformation, temperature or concentration fields of typical multiphysics applications. The performance of the new phase field formulation of fracture is demonstrated by means of representative simulations of failure in metals, rubbery and glassy polymers.

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Oral presentations

Mechanisms for Plastic Flow Localization

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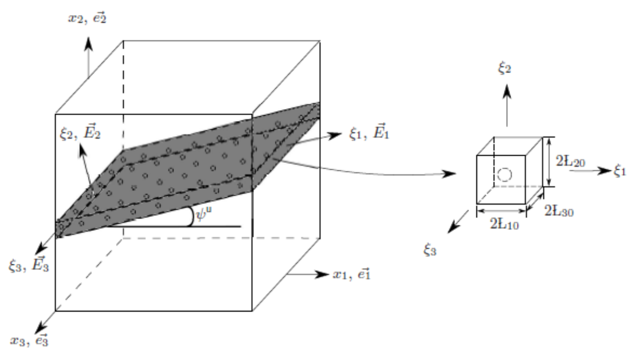

Fig. 1: A weak band containing doubly periodic arrays of voids surrounded by semi-infinite blocks of uniform material. The band is model by a 3D cuboid unit cell containing a void at its center.

The main goal of this study is to understand the relationship in a porous elastoplastic material between macroscopic and microscopic localization of plastic flow at the scale of the ligaments between voids, e.g., the distinction between shear band localization and coalescence between voids. For this purpose, Marciniak-Kuczynski (MK) [1] type localization analyses are performed on 3D unit cells. The standard MK model assumes three regions: two semi-infinite blocks of uniform material having identical properties separated by a band (i.e. and infinite layer) of uniform thickness and uniform properties, see Fig. 1. The band is assumed to contain doubly periodic arrays of voids in the ξ_1 and ξ_3 directions. The infinite block is subjected to a triaxial state of stress with $\sigma_{22} \equiv \sigma_{I} \geq \sigma_{33} \equiv \sigma_{II} \geq \sigma_{11} \equiv \sigma_{III}$, where σ_{I}, σ_{II}, σ_{III} are the principal stresses. For the loading considered, the normal to the plane of the localization band remains in the $\xi_1 - \xi_2$ plane and perpendicular to the ξ_3 axis in the entire course of loading, while the orientation angle of the band evolves with the deformation of the outer blocks.

As shown in Fig. 1, the band is modeled by a 3D unit cell containing a void at the center, see also [2]. The boundary conditions on the unit cell are determined by imposing continuity of tractions across the interface between the outer blocks and the cell. A parametric study is performed to investigate the effects of the initial orientation angle of the band, ψ^u, stress triaxiality, T, Load parameter, L, etc. on the competition between macroscopic localization of plastic flow and the coalescence of voids.

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Crack Thickness and Volumetric Work of Fracture

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Computer modeling of crack propagation requires the knowledge of the *crack thickness* – the width of the damage localization zone, h. To find it we introduce the concept of the *volumetric work of fracture*, ω, which means the amount of energy that should be dissipated by the infinitesimal material volume during fracture. Besides, we use the Griffith concept of the *surface work of fracture*, γ, which means the amount of energy that should be dissipated by the infinitesimal material surface during fracture. Equating the two works of fracture for the representative volume and surface, $\omega h^3 = \gamma h^2$, we find the crack thickness: $h = \gamma/\omega$. We show how to apply the described approach to soft rubber, ductile steel, and brittle concrete. Particularly, we find estimates of the crack thickness for natural rubber [1]: h ~0.2 mm; DH36 steel [2]: h ~10 µm; and plain concrete [3]: h ~2 cm.

Then, we critically discuss the ways to incorporate the characteristic length into numerical simulations including: (a) fixed size of the finite element mesh; (b) nonlocal gradient type theories; (c) nonlocal integral type theories; (d) mesh-dependent constitutive equations. Finally, in view of the significant difference between the length scale of atoms and the length scale of the damage localization zone, we argue that macroscopic fracture is a phenomenon of *emergence* which cannot be predicted based on the knowledge of behavior of individual atoms. Thus, the applicability of *reductionism* to fracture mechanics is questioned.

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A Fracture Criterion for the Notch Strength of High Strength Steels in the Presence of Hydrogen

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High strength steels can suffer from a loss of ductility when exposed to hydrogen, and this may lead to sudden failure. The hydrogen is either accommodated in the lattice or is trapped at defects, such as dislocations, grain boundaries and carbides. The challenge is to identify the effect of hydrogen located at different sites upon the drop in tensile strength of a high strength steel. For this purpose, literature data on the failure stress of notched and smooth steel bars are re-analysed; the bars were tested over a wide range of strain rate and hydrogen concentration. The local stress state at failure has been determined by the finite element (FE) method, and the concentration of both lattice and trapped hydrogen is predicted using the Oriani's theory along with the stress-driven diffusion equations. The experimental data are rationalised in terms of a postulated failure locus of peak maximum principal stress versus lattice hydrogen concentration. This failure locus is treated as a unique material property for the given steel and heat treatment condition. We conclude that the presence of lattice hydrogen increases the susceptibility to hydrogen embrittlement whereas trapped hydrogen has only a negligible effect. It is also found that the observed failure strength of hydrogen-charged smooth bars is less than the peak local stress within the notched geometries. Weakest link statistics are used to account for this stressed volume effect.

Ductile damage model for metal forming simulations including physics based modeling of void nucleation

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A state-of-the-art model of metal plasticity, suitable for metal forming simulations, should account for numerous nonlinear phenomena. If the residual stresses and the spring-back are of particular interest, such model should include the isotropic expansion/contraction and kinematic translation of the yield surface in the stress space. For some metals, however, the influence of the ductile damage induced by plastic deformation should be taken into account, as well. In this work, a model of finite-strain viscoplasticity [1], which was developed by the authors, is extended to ductile damage in a thermodynamically consistent manner. In particular, the interaction between the damage and the strain hardening/softening is captured by the model. It is known that the mechanisms of the isotropic and kinematic hardening are not identical. Therefore, for increasing ductile damage, the ability of the material to exhibit isotropic and kinematic hardening deteriorates differently, as well. Concerning the coupling in the opposite direction, the accumulated plastic anisotropy has a clear impact on the rate of damage accumulation upon the strain path change.

The original model of viscoplasticity is covered as a special case, and the well-established numerical techniques (cf. [1]) still can be used. The model is formulated as an open framework, suitable for further extension. Suitable variants of constitutive relations for void nucleation, growth, and coalescence can be implemented. The restrictions imposed on these relations by the second law of thermodynamics are obtained in an explicit form.

A new law of void nucleation is formulated for porous ductile metals with second phases. This evolution law contains dependencies on the second and the third invariants of the (effective) stress deviator. The corresponding material parameters allow a clear physical interpretation, since the model is based on consideration of different physical mechanisms, like debonding of second phase particles under tensile and shear loading, as well as crushing of the particles under the high hydrostatic stress. The material model is validated using the experimental data on void nucleation in A356-T6 aluminum alloy [2].

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Overview of Peridynamic Theory: Past and Present

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Peridynamic theory is introduced to overcome the problems that the classical continuum mechanics confronted during the existence of the discontinuities in the structure, such as cracks. In this new formulation, equation of motion of a material point is expressed in terms of an integro-differential equation rather than a partial differential equation. Hence, this new form of equation is valid regardless of discontinuities. Furthermore, it has a non-local character, so that the material points which are located at a finite distance can also interact with each other.

The original formulation of peridynamic theory, known as "bond-based peridynamics, is based on pairwise interactions between material points. This assumption results in limitations on material properties that can be used. Today, with the introduction of "state-based peridynamics", any material behavior can be modeled by using peridynamics. Moreover, the non-local character of the theory allows its usage for the structures at the nano-scale to capture the atomistic effects.

Another important improvement on peridynamics has been done through extending the theory to other fields including thermal, electrical, etc. Hence, it becomes a single-platform for multi-physics simulations including superior failure analysis capability.

In this presentation, an overview of peridynamics starting from its origins and its evolution over time will be demonstrated to inform researchers of Europe about this new and exciting continuum theory.

The scale transition procedure for constitutive equations in multilevel models based on crystal plasticity

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Theoretical and experimental studies show that the state of the internal material structure determines the material behavior at the macro level and its physical and mechanical characteristics. Last 20 years models using crystal plasticity, explicitly describing the evolution of the material structure and considered the physical mechanisms of deformation at crystallite level (meso level), are developing very intensively.

One of the keynote questions in the multilevel models construction is the issue of the coherence of constitutive equations at various scale levels. The logical understanding of the problem as follows: macro level relations should be defining from meso level constitutive equations with a priori ties of the macro- and meso level parameters [1]; specific type of ties associated with the aggregation hypothesis (combining elements of meso level to the macro level element). For example, for statistical crystal plasticity models a priori tie is the equality velocity gradient, stresses and the effective elastic properties tensor at the macro level are average the corresponding meso level characteristics (for the velocity gradient this conditions are automatically done because of using Taylor's hypothesis). The relations between other parameters of the macro- and meso level follow from this constitutive equation scale transition procedure (for statistical models thus obtained relations for the inelastic strain rate at macro level and the spin, which determines the quasi-solid motion at macro level).

So the approach leads to concrete form of the constitutive relation at the macro level (in particular the form of corotation derivative of stress), and the relations of low-level "transiting" to the upper-level. In this case, we cannot avoid the phenomenological relations in the construction of models, however, the phenomenological relations are written for the lowest scale level in the models scale hierarchy, for which the specification of physical mechanisms of deformation and a detailed description of them by using the solid-state physics is possible. The proposed method is easy to use for other forms of constitutive relations at meso level and macro level for a wide class of constitutive models with internal variables.

Many existing models [2] not considered explicitly the defining constitutive equations at macro level. However, in the numerical FEM implementation in ABAQUS macro scale level is introduced and the Jaumann derivative of the Cauchy stress tensor is used, which generates incompatibility in the two-level mathematical model . It was shown that this approach could lead to physically incorrect results of simulations.

Two-level model with a description of viscoplastic dislocation slip and grain boundary sliding, lattice rotations with an explicit account of incompatibility dislocation slip in neighboring grains [1] and fragmentation is proposed. With this model different loading schemes of polycrystalline metals are simulated in ABAQUS.

This work was supported by RFBR (grants №12-08-33082-mol_a_ved, №12-08-01052-a, №12-01-31094-mol_a, 13-08-00320-a, 13-01-96006-r_ural_a), the President Grants №МК-3989.2012.1, № МК-390.2013.1.

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Structure Residual Life Assessment with Fatigue Process Specific Accounting

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For a structure lifetime estimation it is necessary to have a knowledge about mechanism of changes in physical-mechanical properties of material under fatigue.

Usually, researchers consider fatigue as a gradual process of damage accumulation under cycle loading that allows them to apply Miner's rule or modify theories for theoretical lifetime estimation. In many researches for the material current state estimation are used characteristic of residual durability (n_2) after prior loading (n_1) that were obtained under two-stage loading. It was noted test results data scattering.

In National Aviation University since 1970's two-stage fatigue tests for different metals and alloys: pure cooper, 12H18N10T and 08kp steels, AD1 aluminum and D16T & 2024-T3 aluminum alloys in statistic aspect (200...300 specimens for each material) are carrying out.

As example, in Fig. 1 the correlation diagram of 12H18N10T steel under two-stage loading is shown.

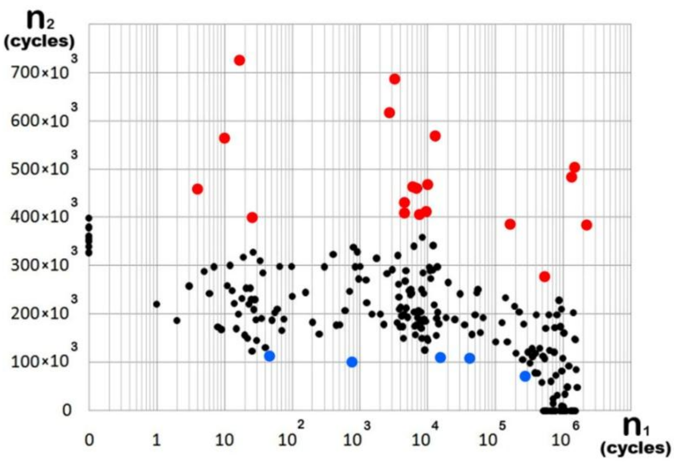

Fig.1: Prior cyclic loading (n_1) vs. residual durability (n_2) diagram

Analyzing the fatigue test results it has been developed synergetic discretely-likelihood fatigue model that based on next ideas [1]:

- there is no reason to search any regression models for the "prior cyclic loading – residual durability" data (coefficient of determination R^2=0,023…0,24) because it will lead to significant errors during calculations.

- metals fatigue process should be considered as a composition of two processes: high-frequency process on a nanoscale and low-frequency that is proceeding on meso- and macroscales;

- high-frequency process is caused by fatigue process bifurcation points in various crystallographic planes. It is characterized by spikes of the residual durability (red points on Fig.1) position of which is described by V. Ivanova recurrent relation;

- low-frequency process is connected with material substructure evolution at various fatigue damage stages and characterized by local minimum with significant residual durability decreasing (blue points on Fig.1);

- there is close relation between spikes bifurcation position ($n_{1\Lambda}$), adjusted value of shear stress τ and grain orientation.

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Viscoelasticity and High Buckling Stress of Dense Carbon Nanotube Brushes

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We report on the mechanical behavior of aligned multiwall (2-4 walls, 1-3 nm diameter) carbon nanotubes (CNTs) produced by non-catalytic vacuum disproportionation of SiC. There is no spacing between the tubes in these brushes, leading to about ~10 times higher density compared to CNT brushes produced by catalytic CVD. Spherical nanoindentation and micro-compression experiments demonstrate a significantly higher loading modulus (~20 GPa) and orders of magnitude higher buckling stress in these dense brushes, as compared to CVD nanotubes or carbon walls. Indentations using indenters of varying sizes show a considerable increase in the buckling strength values with decreasing indenter radii. SEM *in-situ* micro-compression experiments also demonstrate a significantly higher buckling strength for pillars with smaller diameters, suggesting a lower concentration of flaws. We also demonstrate the viscoelastic behavior, caused by the increased influence of the van der Waals interactions between nanotubes, showing their potential for energy-absorbing applications.

Transferability of brittle fracture properties for different specimens and prediction of fracture toughness for RPV steels

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The main aim of the present report is to consider an applicability of two brittle fracture models, namely the Prometey model and the Beremin model, for two issues. These issues are:

- transferability of test results from smooth and notched round bars to fracture toughness specimens of different types, namely CT specimens, SEB specimens with and without side grooves;

- description of the temperature dependence of fracture toughness, $K_{JC}(T)$, for RPV materials with different embrittlement degrees.

It is shown that the Prometey model based on the stress-and-strain controlled local fracture criterion provides adequate results for prediction of brittle fracture for all types of the considered specimens (smooth and notched bars, CT, SEB) from RPV materials with different degrees of embrittlement.

At the same time when using the Beremin model based on the stress-controlled local fracture criterion the transferability of test results between smooth bars, notched bars and fracture toughness specimens is possible only fore case when artificial dependence $\sigma_u(T)$ is introduced. Moreover the Beremin model does not allow adequately to predict the difference in fracture toughness for CT and SEB specimens.

It is shown that small size specimens (for example, SEB-10) overestimate fracture toughness as compared with CT specimens with thickness equal or larger than 12.5 mm. That's why for determination of the temperature dependence of fracture toughness $K_{JC}(T)$ on the basis of small size specimens and application of this $K_{JC}(T)$ for structural integrity assessment of RPV, some margins should be introduced. In frame of this work the values of these margins for RPV steels have been determined on the basis of the calculative and experimental results.

The prestrain effect on brittle fracture: physical features, mechanical modeling and application for RPV steels

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At present, there are sufficiently many experimental results that show different effect of prestrain on brittle fracture. For example, it is known that pretension results in increasing the brittle fracture stress if pretension and subsequent tension occur in the same direction. However, it is found that if subsequent loading occurs in the direction normal to pretension direction the brittle fracture stress decreases [1, 2]. The same finding is revealed for tension after precompression: the brittle fracture stress decreases [3, 4]. Moreover for this case the fracture mode varies from transcrystalline cleavage fracture to intercrystalline brittle fracture [3, 4].

The effect of preliminary loading on fracture toughness K_{JC} may be also different. If cracked specimens are machined from samples undergone pretension on the value ε_0 the dependence $K_{JC}(\varepsilon_0)$ is non-monotonic: it may be increasing and decreasing that depends on ε_0 [5]. At the same time it is well known so-called warm pre-stressing effect: if cracked specimens are undergone preliminary loading at some temperature then at lower temperature K_{JC} always increases. For the same or higher temperature K_{JC} does not practically change as compared with fracture toughness for initial specimens (no preliminary loading) [6].

The purpose of the present report is the physical-and-mechanical analysis of the prestrain effect on brittle fracture properties for reactor pressure vessel (RPV) steel. The report considers the prestrain effect on brittle fracture of RPV steels from viewpoint of

(i) mechanisms of microcrack nucleation and propagation;

(ii) local brittle fracture criterion and the dependence of the critical parameters on prestrain;

(iii) fracture toughness prediction for RPV steels.

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Crack-like defects in welded joints - heterogeneity and constraint effects on fracture behaviour

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Fracture of high-strength low-alloyed (HSLA) steel welded joints is analysed using local approach. The joints were fabricated with one (overmatched - OM or undermatched - UM) and two weld metals; the latter, double mismatched, consist of overmatched and undermatched portion. For most of the specimens, the pre-crack was located in the middle of the weld metal. Therefore, the influence of the material heterogeneity, joint geometry and the position of the crack front is analysed. For some of the specimens, the pre-crack was in the heat affected zone (HAZ). Understanding the fracture behaviour of this zone is especially important bearing in mind often occurrence of micro-cracks and other defects. For the specimens used for comparing the fracture resistance of HAZ and WM, true stress - true strain curves for the welded joint regions were determined by a combined experimental-numerical procedure, utilizing ARAMIS stereometric strain measurement system (www.gom.com) and finite element modelling of smooth tensile panel.

The complete Gurson model (CGM) is applied for modelling of damage development in the material. Its important property is that critical damage parameter value (used as failure criterion) is not a material constant, but depends on the stress and strain state in the structure. This is especially important in the examined joints, where the material heterogeneity causes severe stress and strain gradients. Finite element software package Abaqus (www.simulia.com) is used, with CGM user subroutine UMAT developed by Z.L. Zhang. Influence of the joint width, crack length, crack position and size/formulation of the finite elements in the ligament, is examined. A significant difference in appropriate finite element sizes is obtained for OM and UM weld metals, even though their microstructural parameters are similar. The effect of material inhomogeneity along the crack front of the double mismatched joint is assessed by transferring the parameters from joints with one weld metal. Analysis of the results obtained by testing the same joints with a pre-crack in WM or HAZ revealed the higher fracture resistance of HAZ, as well as significant difference in appropriate element sizes between the WM and HAZ.

Towards Development of Hydrogen Embrittlement Resistant Steel Alloys

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Keywords: Martenstic Steel, Dislocation-Densities, Hydrogen Embrittlement

One outstanding technological problem yet to be solved is the localization and failure of high-strength steel alloys due to hydrogen embrittlement. Hydrogen atoms affect the dislocation core causing the plastic deformation to localize and thus to decrease the material capacity for plastic deformation. Better understanding of the role of the hydrogen will result in reliable computational models that incorporate hydrogen effects and diffusion through dislocation-densities evolution laws.

A molecular dynamics simulation and three-dimensional multiple-slip dislocation-density-based crystalline formulation, specialized finite-element formulations, predictive failure models, and infinity-power integrable function based Voronoi tessellations adapted to martensitic and austenitic microstructure, were used to investigate dislocation density evolution in martensitic and austenitic steel microstructures with and without the presence of Hydrogen.

The interrelated effects of microstructural characteristics, such as variants distribution, arrangement and size, retained austenite and initial dislocation-density, and defects, such as microcracks, and microvoids, were investigated relative to hydrogen presence. The study suggests new hydrogen-embrittlement-resistant high strength steel alloys.

Investigation of Creep-Fatigue Interaction in G91 martensitic steel at 400°C

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The life time of current nuclear power plants was designed to 40 years. Nowadays this limitation is more and more extended towards 60 years. New reactor concepts have already been requested to design for 60 years. Therefore the prediction model of creep-fatigue should be up dated accordingly. The development of models based on short term experiments need large amount of data with low uncertainties to ensure validity. 9Cr1Mo martensitic steel or Grade91 is a high strength steel and provides good creep and fatigue resistance at high temperature. It has therefore been considered as a promising candidate for structrural material in advanced reactor systems. The material needs to be studied in detail in order to realize a safe and economic design. During operation creep damage are usually not occurring alone but together with other damage such as fatigue. Creep-Fatigue interactions are still an ongoing research topic and not yet fully understood. It is known that the presence of both damage mechanisms can drastically reduce the life time compared to the single damage mode. Such coupling could affect the boundary temperature of the negeligible creep domain. However data on creep, fatigue and creep-fatigue interactions for Grade91 steel exists mainly at high temperature and below 450°C data is scarce. The goal of this project is to study creep, fatigue and their interaction at 400°C. Creep experiments were done at different stresses with flat dog bone samples. Creep-fatigue experiments were conducted with cylindrical dog bone samples in strain controlled mode for the cycling and stress controlled mode for the holding times. Damage assessment was done based on the linear damage accumulation rule which is accepted for G91 steel by ASME. Finally the impact of present results on prediction model is discussed by comparing together with literature data at low temperature region.

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Experimental and Computational Investigation of Dynamic Crack Growth along Curved Interfaces

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Failure of curved weak interfaces is important in bonded joints, curved composite laminates and earthquake faults. Crack growth in curved weak interfaces may occur dynamically as a result of curvature and loading even under quasi-static loading conditions. In this paper, dynamic crack growth along curved interfaces under quasistatic loading is investigated experimentally and computationally. The effect of initial crack length on the stability of the crack growth is examined. In the experimental study, a unique testing fixture with a sliding platform is designed to create a displacement loading perpendicular to one of the arms in a curved beam. The full-field techniques of digital image correlation and photoelasticity are used in conjunction with a high speed camera in order to visualize stress and strain fields around the interface crack. In the computational study, debonding at the interface of the curved interface is modeled using dynamic (explicit) finite element analysis in conjunction with Xu-Needleman cohesive zone model with a pure vertical displacement loading to reflect the same loading condition as the experiment. Experimental and finite element analysis results are found to be in agreement in terms of load-displacement behavior, stress distribution, and crack tip speeds. Stable and unstable crack growth regimes, depending on the pre-crack length, are identified in agreement with energy release rate calculations. In the unstable crack growth regime, crack tip velocities at the material wave speeds are observed.

XFEM applications for integrity analysis of Reactor Pressure Vessels cracked walls

Vicente Francisco González Albuixech, Qian Gian, Markus Niffenegger

The structural integrity analysis of a Reactor Pressure Vessel (RPV) related to Pressurized Thermal Shocks (PTS) has been widely studied. This analysis involves the comparison of the mode I stress intensity factor (K_I) for the assumed crack with the fracture toughness of the material (K_{IC}). However, due to the difficulties associated with the building of a 3-D finite element model. The K_I computation is usually limited to simple geometries and crack configurations. In the last years new methods appeared that make the computational fracture mechanics studies of more complex models feasible. One of those methods, the eXtended Finite Element Method (XFEM) relies on the introduction of the crack effect with an enrichment of the finite element approximation space. Furthermore, XFEM has been recently implemented in the commercial code ABAQUS making it available for the applied structural analysis.

Although XFEM is accepted as mesh independent, it shows some minor drawbacks that impose some limitations to its application. XFEM enrichment corresponds to a planar crack with a straight crack front and uses level sets for crack description. Consequently in order to reproduce the effect of a given curved or non-planar crack the mesh should be refined enough to capture and describe the crack topology and influence. One of the approaches widely used for the SIF computation is the domain integral method. The XFEM implementation of domain integral method accuracy is affected by the relationship between mesh and crack topology. Hence, the domain integral should be calculated carefully in XFEM.

In this study, we will outline some of the problems associated with the ABAQUS XFEM fracture mechanics approach and also how to minimize or avoid its effects. In order to show the advantages of the XFEM, and the real applications possibilities, we also present preliminary results of the XFEM applications to the structural analysis of a cracked RPV subjected to a PTS load.

Strain-induced damage of metals under large plastic deformations

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One of the main problems in damage mechanics is still a formulation of a thermodynamically consistent theoretical framework for strain-induced damage of metals. The development of such a theory for ductile damage under large plastic deformations allows us to use it efficiently for the modeling and engineering calculations of metal forming processes. The appropriateness of the tensorial damage model for the process analysis is based on experimental studies of void growth and coalescence under large plastic deformations [1-3].

A high-quality meso-structure of metals essentially improves their ability to withstand dynamic impact loads and also enhances their fatigue resistance. Void coalescence can lead to large cavernous defects and clusters and, consequently, to a “drop” in operating performance of metallic components subjected to high temperatures, pressures, and strain rates which are typical for aerospace, automotive and energy engineering applications. The development of such metal forming procedures that can provide the absence of void coalescence is very important and, in some cases, necessary for metalware industry.

Based on a micromechanical concept of the void volume growth and a change of the void shape the dissipation potential and constitutive equations for ductile damage of metals are presented. Multiplicative decomposition of the metric transformation tensor and thermodynamic formulation of the constitutive equations lead to a symmetric second order tensor of damage which is physically meaningful. Its first invariant defines the damage related to plastic dilatation of the material due to the void growth. The second invariant of the deviatoric tensor accounts for the damage associated with a change in the void shape.

Two physically motivated normalized measures of damage are introduced. They allow us to represent the kinetic process of strain-induced damage by using the equivalent parameter of damage including the limit conditions for the onset of void coalescence and ductile failure. Two measures of ductile damage can be useful when assessing the quality of the meso-structure of metallic components produced by forming processes. An experimental analysis of the evolution of ductile damage is presented for the case of uniaxial tension and compression of metallic specimens with artificial defects.

KEY WORDS: Void, Coalescence, Large Deformation, Damage, Ductile Fracture, Metal Forming

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Comparing two models for slip-patterning and strain-localization based on a non-convex plastic energy

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Keywords: Martenstic Steel, Dislocation-Densities, Hydrogen Embrittlement

In this paper, two different strain gradient plasticity models based on non-convex plastic energies are presented and compared through numerical experiments. Both models are based on the additive decomposition of the strain into elastic and plastic parts. The difference arises from the evolution of plastic deformation.

The first model, proposed in [1], follows the principle of virtual work to get balance equations and the dissipation inequality, in order to obtain the plastic evolution equation. The free-energy is given by the sum of a non-convex plastic term, and two quadratic terms with respect to the elastic deformation and the plastic deformation gradient. The resulting model is rate-dependent, and it accounts for processes where the plastic deformation is partially recoverable.

In the second model, developed in [2], the plastic evolution is determined by incremental minimization of an energy functional which is equal to the free-energy of the above model (sum of a non-convex plastic term, a quadratic elastic term, and a non-local term). In this case, the plastic term is supposed to be totally dissipative. Therefore, plastic deformations are not recoverable. The resulting framework is rate-independent, contrary to the first model.

The two models are implemented by finite elements, and two one-dimensional problems are solved. In the first one a double-wells plastic energy is considered, and the evolution of slip patterns in crystals is reproduced. In the second problem a convex-concave plastic energy is used to simulate the response of a tensile steel bar, where plastic strains localize up to fracture. In this way different inelastic phenomena are captured by assigning different shapes to the plastic energy. The numerical examples exhibit good agreement between the two models. The solutions provided by the rate-dependent model approach those of the rate-independent model, as the imposed deformation rate reduces.

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Influence of hydrogen on dual phase steel deformation micro-mechanics

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Among the advanced high strength steels introduced in the last decades, dual-phase steels, which combine relatively easy processing with excellent mechanical properties, are the first to be employed in the automotive industry. While it is known for decades that the composite-like martensitic-ferritic microstructure is responsible of the observed combination of high strength and good ductility, the extent of the strain and stress partitioning at the microstructure scale is only recently being investigated with the advent of proper in-situ testing techniques. The micro-mechanics of hydrogen embrittlement phenomena in DP steels, on the other hand, is still not sufficiently investigated. Currently available reports typically resort to analysis of macroscopic behavior in presence of hydrogen (which strongly underlines the susceptibility), while the connection to the underlying deformation mechanisms is limited. It should also be noted that the weak link to the underlying microstructure is partially due to the difficulty of in-situ testing of hydrogen charged samples (i.e. due to desorption effects).

In this work, we aim to improve the understanding of hydrogen embrittlement phenomena in DP steels. For this purpose, tensile deformation experiments are carried out with and without cathodic hydrogen-charging, and the resulting macroscopic behavior and the deformation microstructures are comparatively analyzed. For microstructure characterization, different scanning electron microscopy based-techniques are employed, e.g. electron channeling contrast imaging, electron backscatter diffraction, etc. Furthermore, in-situ bending experiments are carried out with and without hydrogen-charging, where light microscopy imaging is employed to minimize hydrogen desorption-induced complications. Obtained results reveal a strong influence of hydrogen on the elongation to failure. Analyses of the deformed microstructures reveal that this decrease is related to microstructural damage evolution triggered at very low deformation levels (~2%), while strain partitioning between martensite and ferrite is not significantly affected. In-situ experiments reveal the cause of enhanced damage nucleation to be martensite-ferrite phase boundary weakening. Ongoing analyses are underway to reveal the extent of hydrogen partitioning between the two phases.

Posters

Stress-deformable state of isotropic plate with four non-through cracks and a circular hole

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Keywords: non-through crack, circular hole, stress intensity factor, Line-Spring Model, method of boundary integral equations.

Today thin plates of different configurations are widely used in modern technology. The wear of those details is characterized by small damages, fractures, cracks, cuts, etc. These defects often play a significant role in the deterioration of the material properties and the carrying capacity of structures, and, therefore, the structures are less reliable, especially, if they have a lot of defects.

Therefore, a necessity in research of the stress-deformable state of plates in order to study the quality of the construction strength with cuts is appeared. Obtaining load distribution in the vicinity of the cut allows analyzing the stress state of the plate with defects, increasing the age of constructions and changing the safety factor at the same time.

Thus, the stress concentration of the cut in a structural element (in the particular case - the plate) is one of the problems for fracture mechanics.

A thin isotropic elastic plate of constant thickness *h* is considered in the research. The coordinate system is chosen in such a way that the axes *x, y* are oriented along the directions of plate elastic symmetry. The plate is weakened by four cross non-through (internal) cracks of different length, directed along the axes, and by a circular hole of radius *R*, located in the center of the construction (Fig. 1). The plate is subjected to external balanced load - uniform tension along the *y* axis. To solve this problem we applied the following methods: integral Fourier transform, the theory of generalized functions, the method of boundary integral equations, the Line-Spring Model and the method of mechanical quadratures. The numerical solution shows each other defects effect while they are close together.

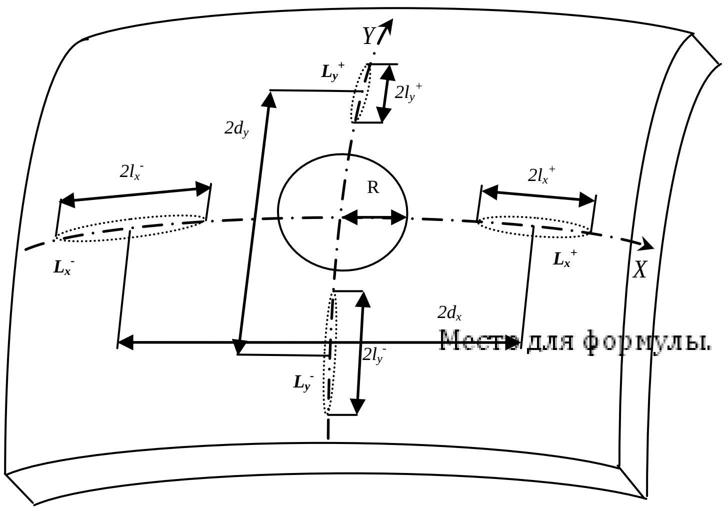

Fig. 1. Plate with defects

Structural reliability approach in thermal fatigue crack growth by stochastic modeling

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The problem of thermal fatigue in mixing areas arises in nuclear piping where a turbulent mixing or vortices produce rapid fluid temperature fluctuations with random frequencies. The assessment of fatigue crack growth due to cyclic thermal loads arising from turbulent mixing presents significant challenges, principally due to the difficulty of establishing the actual loading spectrum. To apply the stochastic approach of thermal fatigue, a frequency temperature response function is proposed. For the elastic thermal stresses distribution solutions, the magnitude of the frequency response function is first derived and checked against the prediction by FEA. The connection between SIF's power spectral density (PSD) and temperature's PSD is assured with SIF frequency response function modulus. The frequency of the peaks of each magnitude for KI is supposed to be a stationary narrow-band Gaussian process. The probabilities of failure are estimated by means of the Monte Carlo methods considering a limit state function.

Mathematical Analysis of Cracks Interaction in Anisotropic Materials

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Crack initiation at a crack tip, propagation direction, cracks tip fields and cracks interaction in static orthotropic plane linear elasticity are the main themes for mathematical modeling and simulation and represent important problems of Fracture Mechanics.

We consider one, two or three collinear cracks in an anisotropic material subjected to mode I and II of Fracture Mechanics.

Our first aim is to determine the elastic state produced in the body using complex potentials. We use Lekhnitskii representation theorem of the stresses and displacements fields with complex potentials. We give the boundary conditions which must be satisfied by the complex potentials on the faces and at large distances from the cracks. Using the theory of the Riemann-Hilbert homogeneous and non-homogeneous problems, Plemelj's function and Cauchy's integral we obtain the general solution of our complex potentials.

Assuming that our applied uniformed normal applied stresses, and in second case, tangential stresses have constant value, we give an explicit solution of our mathematical problem.

Our second aim is to determine the asymptotical behavior of the stresses and displacements fields in a vicinity of the cracks tips. To do this we determine first the non-regular or asymptotical values of the complex potentials. The obtained results are important in a future research to determine the energy release rate and strain energy density for each tip of the cracks. In that moment we are able to study the cracks interaction, using numerical methods and later on, to validate these results with experimental tests which will be performed on particular types of anisotropic elastic composites.

We consider as an example two configurations of two and three equal and collinear cracks in a Graphite-epoxy fiber reinforced elastic composite. Using numerical analysis we determine that:

- in the case when the distance between the cracks is much smaller than their length, *i.e.* there exist a strong interaction between the cracks, first start to propagate the inner tips of the cracks and cracks tend to unify;

- in the case when the distance between the cracks is much greater than their length, *i.e.* there exist a weak interaction between the cracks and all cracks start to propagate almost in the same time.

Integrity analysis of a reactor pressure vessel subjected to pressurized thermal shocks by considering constraint effect

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Keywords: pressurized thermal shock, constraint loss, reactor pressure vessel, fracture mechanics

The integrity of a reactor pressure vessel (RPV) related to pressurized thermal shocks (PTS) has been extensively studied. However, the study on the variation of T-stress along the crack-front (crack tip constraint loss) of a surface crack in a RPV subjected to PTS is lacking. This paper introduces the method of using fracture mechanics for the integrity analysis of a RPV subjected to PTS transients. A 3-D finite element model is used to perform thermal and fracture mechanics analysis by considering both elastic and elastic-plastic material models. The elastic-plastic effect of the material is also analyzed by the plastic zone size of the crack tip. The results show that the linear elastic analysis leads to a more conservative result than the elastic-plastic analysis. A shallow crack is assumed in the RPV and the corresponding constraint effect on fracture toughness of the material is quantified by the K-T method. The stress intensity factor (SIF) for the deepest point of a surface crack is not always larger than that for a surface point, indicating that both the deep and surface points of the crack tip should be considered in the integrity analysis. Subjected to the medium loss-of-coolant accident (MLOCA) transient the crack tip has a constraint loss. The safety margin of the RPV is larger based on the K-T approach than that based on a Konly approach.

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Effective Spring Stiffness for the Interfaces between Dissimilar Solids Weakened by Periodic Array of Cracks

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An effective spring stiffness formulation is proposed for the interface between two dissimilar solids weakened by the array of collinear and coplanar interface cracks. The formulation for collinear slit cracks is derived exactly and coplanar penny-shaped cracks approximately. The approximate form is derived based on the approximation where the influence of crack interactions on strain energy release rate are assumed to be same for interface cracks and cracks in homogenous media. The validity of this assumption is proved for split type interface cracks and this assumption can be used for penny-shaped cracks by knowing that it will lead even less error because the interaction effect is less in coplanar penny-shaped cracks compared to collinear slit cracks. This assumption allows factorization of spring stiffness expression into the material dissimilarity factor, the crack interaction factor and the effective spring stiffness solution for non-interacting cracks in a homogeneous material.

The crack interaction factor is obtained using a recently developed model for stress intensity factors for an array of coplanar penny shaped cracks in a homogeneous material; also the material dissimilarity function recently obtained for non-interacting penny shaped crack at the interface between two dissimilar materials is employed. The obtained solution is useful for an assessment by ultrasonic measurements of the interface stiffness in bonded structures for monitoring the interfacial microdamage growth due to mechanical loading and environmental factors.

Two-level models of polycrystals: investigation of hardening laws influence on the macro effects of complex cyclic loading and damage accumulation

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Changes in the physical and mechanical properties of the specimen during deformation in complex cyclic path is a consequence of a substantial restructuring of the micro- and mesostructure of the material, mainly - due to a significant evolution of the dislocation (wider - defective) material structure. Describing such processes is impossible without studying and establishing appropriate mathematical models that explicitly take into account the physical root causes of the microstructure evolution of the material under large deformations and can be applicable to the description of damage accumulation and fracture processes. The foregoing explains the considerable attention in crystal plasticity, which is paid to the modification of hardening laws.

The goal is to study the effects produced by polycrystalline material under proportional and non-proportional cyclic loading (and the transition from one to another type of loading) as a consequence of changes occurring at the dislocation structure in the process of loading, and attempt to modify the hardening laws so that they can be transparently physically describe these changes and effects. In particular, there is attempt to justify and describe the known experimental effects, such as the dependence of additional cyclic hardening of the disproportionality of loading, cyclic softening the transition from non-proportional to proportional loading, transverse hardening, which manifests after proportional loading in one direction is followed by proportional loading in the other direction.

We received both general and particular form of hardening laws of mono- and polycrystalline allows describing the formation and destruction of dislocation barriers, the annihilation of dislocations as well as additional hardening, resulting from the interaction of intragranular and grain boundary dislocations. Hardening is divided into "non-oriented" and "oriented". The first type describes the hardening regardless of the direction of deformation (under this definition, processes such as the formation of the intersection of dislocations, plaits, braids, dislocation barriers), and a hardening increases the critical shear stress at once on many slip systems (or even all at once). The second type is related to the accumulation of elastic energy to "pursed dislocations" (at different barrier) and this energy may be (fully or partially) released at the change the direction of deformation. The analysis of the possible mechanisms of interaction between carriers and the plastic deformation of the crystal lattice defects is executed; hardening laws that discovers a good agreement with experimental data are proposed. We also introduce the parameters characterizing the accumulation of damage and formulate fracture criterion using methodology of multilevel modeling.

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A Three Dimensional Model for Nanocrystalline Materials based on Grain Interior and Grain Boundary Deformation Mechanisms

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Nanocrystalline metals, because of their distinct features, e.g., high strength, low ductility, pronounced rate dependence, tension-compression asymmetry and susceptibility to plastic instability, has become the subject of intense research over the past two decades [1]. Owing to a large volume fraction of grain boundary (GB) atoms, the deformation mechanisms in nanocrystalline metals are different from traditional coarse-grained polycrystals. Indeed, there are several inelastic deformation mechanisms, e.g., GB-diffusion, GB-sliding, dislocations, grain rotation, grain growth and GB-migration, which can be simultaneously operative in nanocrystalline metals. In this work, a three dimensional viscoplastic constitutive model for nanocrystalline metals is presented. Different from most constitutive models where nanocrystalline metals are considered as multi-phase composites with corresponding volume fractions, the proposed model does not assume a parameter for a GB-thickness or GB affected zone. The proposed model is an extension of the one-dimensional model originally developed in [2] and is based on several competing grain boundary and grain interior deformation mechanisms. GB-diffusion (Coble creep) [3], GB-sliding [4], and the grain interior dislocation-mediated-plasticity [5,6] are the three different types of deformation mechanisms that are assumed to be operative in this work. The first two micro-mechanisms are GB-based, whereas the last one is related with the grain interior. Effects of pressure on the grain boundary diffusion and sliding mechanisms are taken into account. Furthermore, the influence of grain size distribution on macroscopic response is studied. Finally, the model is shown to capture the fundamental mechanical characteristics of nanocrystalline metals. These include grain size dependence of the strength, i.e., both the traditional and the inverse Hall–Petch effects, the tension–compression asymmetry and the enhanced rate sensitivity.

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Crystal plasticity based prediction of creep and microcracking in irradiated polycrystalline graphite

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Predicting the macroscopic shape changes of irradiated polycrystalline graphite agglomerates requires multiscale modeling. The mechanical response of the aggregate depends, on the one hand, on the interaction of adjacent, highly anisotropic grains with different lattice orientations. The global behavior is, on the other hand, strongly influenced by the opening and closure of microcracks.

A crystal plasticity model is proposed, which incorporates an anisotropic description of thermal expansion, elasticity, irradiation-induced dimensional change and creep at the single crystal level. The model is implemented as a user-defined constitutive law in a finite element code and a cohesive law serves to model crack propagation at the grain boundaries. A model two-dimensional aggregate comprising 100 grains is meshed with finite elements conforming to the grain boundaries and periodic boundary conditions.

The model reproduces the thermal expansion coefficient of polycrystalline graphite, the irradiation-induced dimensional change (initial shrinkage followed by swelling at higher fast neutron fluence) and irradiation creep (including the reduction in creep coefficient at high fast neutron fluence). The predictions agree qualitatively with experimental data. The main discrepancies are likely to be overcome by applying the model to more realistic three-dimensional polycrystals.

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Numerical Investigation of Failure Mechanisms and Energetic Distrubitions in Elastomers at Steady State Crack Propagation

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Keywords: Material force approach, viscoelastic fracture mechanics, elastomers, Initially rigid cohesive zone elements

The failure mechanism in elastomers is of great importance and interest in engineering applications. However, the correlation between numerical and theoretical studies is not well established due to the complexity of the problem. The contribution presents crack propagation scheme and implementation of the cohesive zone interfaces at a frozen time step during the solution process for the description of the viscoelastic fracture response of rubber-like materials at large strains. Key feature of the procedure is restructuring the overall system by duplication of crack front degrees of freedom based on minimization of the overall energy via the Griffith criterion. Previous studies are restricted to small strain elastic materials. Therefore, in this contribution, we aim to extent previous approaches to a generalized finite inelastic continuum. The experimental evidence favors that the fracture toughness of non-strain-crystallising elastomers shows strong rate-dependency and the energy release rate versus the rate of tearing or crack propagation relation appears to be a fundamental material property. A dynamic fracture criterion, which is a function of the rate of crack growth, is shown to be more adequate in numerical simulations. In addition, in previous studies, it is shown that the fracture energy per unit area of crack advancement appears to be the result of two contributions in terms of the change in elastic energy and in terms of the viscous dissipation by a configurational change. The separation of the fracture energy is obtained by global energy momentum balance. To this end, a consistent thermodynamic framework for the combined configuretional motion in viscoelastic continua at the finite strain regime is discussed. The Bergstörm-Boyce model is considered to introduce hyperelastic and finite viscoelastic behaviour of the rubber-like bulk material. In addition to the bulk material, a polynomial function is introduced in order to obtain an initially rigid cohesive zone behavior with a steady state crack propagation scenario in the continuum. The crack driving force and the crack direction are predicted by the material force approach. The predictive capability of the proposed method is demonstrated by representative numerical examples.

The phenomenological model of the fatigue crack growth considering damage accumulation

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Keywords: Martenstic Steel, Dislocation-Densities, Hydrogen Embrittlement

The theoretical approach to the modeling of fatigue fracture based on the joint consideration of boundary-value problem of fracture mechanics and damage kinetics problem of the continuum damage theory is presented. It is assumed that fatigue damage accumulation is the cause of crack motion. Two-stage process damage accumulation involves the incubation stage and crack propagation stage. This process is described by scalar parameter of damage $\omega \in [0;1]$. The condition of the damage parameter equality to 1 is taken as the criterion of the fatigue fracture front initiation and movement. It is assumed that main part of body is deformed linear-elastically while all non-linear effects are concentrated in plastic zones at the crack tip. According to presented model the fatigue crack increases step by step on the length of cyclic plastic zone. The lengths of plastic zones near crack tip are defined on base modified Dugdale model.

The basic relations of the model are obtained from the solution of the non-linear integral equation for fatigue crack front movement. The values of the constants of basic equations of the model are determined from two base experiments. The first group characterizes the plastic behaviour of a material and is determined from stress-strain diagrams in uniaxial tension tests. The second group involves coefficients which characterize the material resistance to the accumulation of scattered fatigue macrodamage and they are calculated by the results of standard fatigue tests of smooth cylindrical specimens under uniaxial reversed tension-compression presented in a form of Wöchler curve.

The model was tested on the solution of the problem of the growth of a central crack in a thin rectangular plate under uniaxial high-cycle loading. The stress distribution in the vicinity of the crack tip is defined by numerical-analytical method that is combined on the complex variable method of Muskelishvili and boundary-collocation method. The calculation results of the dependence of crack length on the number of load cycles agree well with those obtained by experiment.

Strained-Heteroepitaxial Quantum Dots with Anisotropic Surface Properties

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Keywords: Martenstic Steel, Dislocation-Densities, Hydrogen Embrittlement

Semiconductor Quantum Dots' capability to create exciton makes them attractive for the design and fabrication of novel electronic, magnetic and photonic devices. The excitons are spatially confined and their energy spectrum, which controls many physical properties of interest, can be adjusted over a wide range by tuning composition, density, size, lattice strain and morphology. To make use of these features, researches leading to reliable means for estimating forces in small material systems and establishing frameworks, in which the integrity or functionality of the systems is satisfied, are needed. Main technology-limiting barrier is the material failure due to capillary-driven morphological evolution of surfaces and interfaces in condensed matter; especially under the action of applied force fields e.g., electrostatic and thermo-mechanical. In such nano-scale systems, the magnitude of the surface roughness, diffusion anisotropy and texture orientation may have a significant influence on the thin film surface evolution. Here we demonstrate the modeling of formation of semiconductor QDs by manipulating anisotropic material properties (the crystal texture: surface Gibbs free energy, diffusivity) under stress field. A systematic study based on self-consistent dynamical simulations will be presented for the spontaneous evolution of an isolated thin solid droplet on a rigid substrate, utilizing various combinations of the surface texture and the direction. The anisotropic surface free energy and the surface stiffness were treated using well accepted trigonometric functions. Although, various tilt angles and anisotropy constants were considered during simulations, the main emphasis was given on the effect of rotational symmetries associated with the surface Helmholtz free energy topography in two-dimensional space.

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First-principles and quasi-continuum investigations of the material properties of two systems: dispersive-reinforced Al alloys and Ti/H2 system

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Keywords: aluminum alloys, ultra dispersed diamond powder, titanium, adsorption, mechanical strain, binding energy

The purpose of this work is to compare a Quasi-continuum (QC) modeling method with an ab initio approach to study metallic systems for space and energy applications. The goal is assessment of the approaches by desired crtiteria, such as accuracy and applicability, for selected applications.

Composite materials are prevalent in modern aerospace industry and the requirements for them have increased considerably. We designed and tested a new composite material, based on an Al-W matrix reinforced by nano-dispersed diamond powder. This material is desirable for its combination of maximum strength with high modulus of elasticity, heat resistance, abrasion resistance, low density and other properties. In space applications, advanced composites are required to possess capability to function under extreme conditions and to have a series of specific physical and mechanical properties. Thus, the study of this material in outer space conditions is preceded by preliminary simulation studies, using the atomistic approaches. Comparison of the methods QC and MD and/or QC and DFT/ab initio is performed for a chosen small system (e.g. individual dislocation motion, vacancy formation or motion, etc.).

Further investigation is performed on the system Ti/H2 by a DFT/ab initio method for finding appropriate interatomic potentials, as well as by a QC method, for determining surface parameters (such as sticking coefficient, saturation curve, adsorption-desorption boundaries, etc.). The results are compared with preliminary studies on the binding energy characteristics of titanium (Ti) and hydrogen (H2), using an ab initio approach.

The subject of the binding energy of hydrogen on Ti with strains is of significant amount of interest in explaining the hydrogen storage capabilities for fuel cell applications. The current work contributes to determining a strain state with high binding energy for hydrogen input and storage, and alternatively to binding energy strain condition for easy release of hydrogen for combustion in fuel cells.

Assessment of Fracture Initiation point in Inclined notch on Brazilian Disk under Pressure

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Keywords: mixed mode, Equivalent Notch Stress Intensity Factor, Brazilian disk, MTS criterion

Mixed mode fracture emanating from notch has recently received increasing attention. The criterion based on the maximum tangential stress (MTS) criterion for crack are developed for notch problems. The critical tangential stress, expressed in terms of mode I and II notch stress intensity factors, has proposed to an approach based on Equivalent Notch Stress Intensity Factor. This paper is focus on initiation point on fracture emanating from notch using MTS criterion for Brazilian disk made in bio-ceramics. A comparison between U and V notches is made.

Cohesive zone modeling of intergranular cracking in polycrystalline aggregates

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Understanding and controlling early damage initiation and evolution are amongst the most important issues in nuclear power plants, occurring both in austenitic steels and nickel based alloys. A meso-scale approach to modeling intergranular cracking is presented, with explicit account for grain boundaries using the cohesive zone approach. Two cohesive-zone approaches are compared: cohesive surfaces and cohesive elements. Cohesive surface approach is simpler to implement while the cohesive elements make the tracking of the damage initiation and evolution easier. The response under anisotropic elasticity with crystal plasticity constitutive law computed and the stability of the analysis for each of the cases is explored for the two cohesive zone approaches. The approach with cohesive surfaces results in significantly more stable simulations with only a very small amount of viscous regularization required. On the other hand the cohesive element approach exhibited numerical convergence issues even with significantly higher amounts of viscous regularization. The effect of element type is also explored. Linear 4-node tetrahedron elements (ABAQUS types C3D4) exhibited resulted in better stability compared to modified 10-node tetrahedron elements (ABAQUS types C3D10M), while similar crack surface was obtained in both cases, Figure 1.

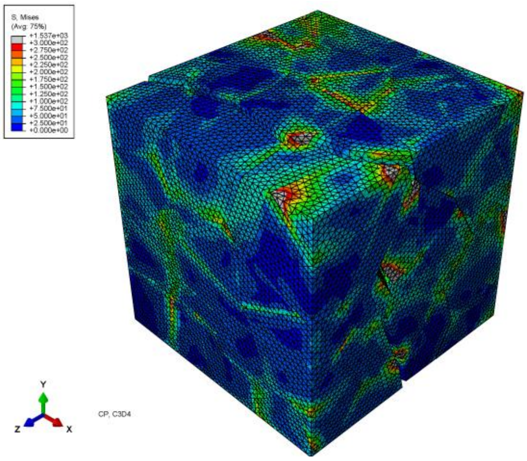

Figure 1. Polycrystalline aggregate with 150 grains and fully developed intergranular crack. Cohesive surfaces are used.

A Polycrystal Approch to Analyse Texture Evolution during Asymmetrical Rolling

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The asymmetric rolling process differs from conventional rolling through the use of different roll circumferential velocities or diameters. Using proper parameters, asymmetric rolling imposes intense shear deformations across the sheet thickness, leading not only to the occurrence of shear texture, but also to grain refinement. In fact, some shear texture components are known to improve plastic strain ratio values, and thus formability.

In this work, the rate-independent polycrystal model of Gambin [1] was efficiently implemented and applied to predict the mechanical response of distinct texture components that appear after asymmetrical rolling. For FCC materials, this polycrystal plasticity model avoids the uniqueness issue related to the choice of the set of active slip systems by applying a regularized Schmid Law. Consequently, it generates yield surfaces with smooth corners where the normal vector is always uniquely defined. Also, it doesn't require the arbitrarily defined reference strain rate commonly used in the viscous-approximation of rate-dependent models.

For validation purposes, a 1050-O sheet was subjected to tensile and shear tests. The model could accurately simulate the measured results. In the end, ideal textures components were simulated and their mechanical response was evaluated. Hence, it is stated a solid basis to justify the improvement of sheet's mechanical properties after asymmetrical rolling when compared to conventional rolling.

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Biomechanical evolution of a novel modular plate, used in spinal surgery

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Keywords: Modular Anterior Lumbar Plate, Iterative Design, In Vitro Test, Fatigue Performance,

In this study, a new type of anterior lumbar plate is designed iteratively. This plate reduces inventory costs and allows various sizes of fixations. The size of the plate can be regulated as needed during the surgical operation whereby using of this design. Studies start with a basic first model which has identical modules. The first design was failed from biomechanical tests carried out according to ASTM F 382 and modified iteratively to that biomechanical test results. ASTM F382 biomechanical tests performed on each new design. Final model was achieved after three iterations. It was considered as safe as a traditional rigid plate in terms of its static and fatigue biomechanical performances and has sufficient quality for using surgical operations.

Polymer Brush Grafted Magnetic Nanoparticles for Highly Efficient Water Remediation

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Highly efficient removal of mercury metal ion (Hg^{II}) from water is reported by employing polymer brushes functionalized magnetic nanoparticles (MNPs). Surface initiated conventional radical polymerization (SI-cRP) was used to grow poly(2-aminoethyl methacrylate hydrochloride) (Poly-AEMA.HCl) polymer chains on magnetite nanoparticles (Fe_3O_4), followed by transformation of pendant amino groups into dithiocarbamate (DTC) groups which showed high chelating affinity towards Hg^{II} ions. This polymer brush based DTC functionalized MNPs (MNPs-Poly-AEMA.DTC) platform showed the complete removal of Hg^{II} from aqueous solutions. The Hg^{II} removal capacity and efficiency of MNPs-Poly-AEMA.DTC were compared with its monolayer analogue. All surface chemical modifications and higher chelating functional group density in case of MNPs-Poly-AEMA.DTC were ascertained by transmission electron microscopy (TEM), thermogravimetric analysis (TGA) physical property measurement system (PPMS), attenuated total reflectance infrared (ATR-IR) spectroscopy, and X-Ray photoelectron spectroscopy (XPS). The Hg^{II} removal capacity and efficiency of monolayer and polymer brushes based DTC functionalized MNPs was evaluated and compared by studying the effect of various factors on Hg^{II} removal percentage such as adsorbent amount, temperature, and contact time. Furthermore the adsorption behavior of MNPs-DTC and MNPs-Poly-AEMA.DTC were analyzed by applying Langmuir and Freundlich adsorption isotherm models. Additionally the adsorption thermodynamics as well as adsorption kinetics were also evaluated in detail. Because of the higher surface functional group density of MNPs-Poly-AEMA.DTC exhibited superior remediation characteristics towards Hg^{II} (>97%) when compared to its monolayer analogue (68-72%).

In-vitro Investigation of Fusion Effect On Pedicle Screws In Terms Of Pullout Strength

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Keywords: Bone Screw, Pullout, Experimental, Osteoporotic and Fusion

Pullout is a very common problem on the use of pedicle screws especially for osteoporotic bones. Much is written about parameters that effect the pullout strength of pedicle screws, for instance screw design and bone mineral density (BMD). In this study, a previously designed pedicle screw was tested experimentally. Fusion (bone in growth) phenomena was simulated for the first time in literature. Healthy, osteoporotic and severely osteoporotic bone like synthetic foams were compared either before and after fusion conditions, respectively, in terms of pullout strength. 70% higher pullout strength was achieved in after fusion condition in osteoporotic bone simulating synthetic foam. Contrarily, no dramatic deviation was considered between before and after fusion conditions in healthy and severely osteoporotic bone simulating synthetic foam.

The Effect of Per-phase Properties on the Ductility of Dual Phase (DP) Steels

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Most of the ductile fracture models in the literature neglect the presence of second-phase particles and make use of phenomenological stress and/or strain controlled void nucleation laws, where the nucleation stress/strain values are defined with respect to the overall values in the material, and not to the local field quantities in the particles or along the particle–matrix interfaces. Moreover, due to a lack of coupling between void nucleation and particle response, even the most advanced fracture models involving homogenization based nucleation laws cannot capture the softening of the material associated with the loss in the load carrying capacity of particles. If, however, the particle volume fraction is typically larger than 5–10 %, neglecting the presence of the particles leads to dramatically poor estimates for the fracture behavior of materials. Recently, a micromechanics based ductile fracture model is developed for composite materials [1]. The model integrates the Gologanu-Lebond-Devaux (GLD) constitutive law for porous plasticity with an enhanced mean-field (non-linear Mori-Tanaka) homogenization theory, and is referred to as the "integrated Mori–Tanaka-damage (IMTD) model". In this study, the IMTD model is employed to investigate the microstructure that will optimize the mechanical response of DP steels in terms of strength/ductility balance. DP steels are modeled as particle reinforced composites. Before proceeding with the fracture analysis, the parameters involved in the Mori-Tanaka scheme are adjusted through comparison with two-dimensional (2D) axisymmetric finite element models for the ferrite-martensite composite. Following this, an extensive parametric study will be performed by using the IMTD model in order to investigate the effects of parameters such as the volume fraction, carbon content, and the critical fracture strength of martensite, and the grain size of ferrite on the mechanical response of DP steels.

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Reliability Estimation of Aircraft Structures Using Tail Modelling

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Reliability of aircraft structures can be estimated via tail modelling. Tail modelling involves performing a relatively small number of limit-state functions using sampling methods such as Monte Carlo Simulation, selecting a threshold to identify the tail and fitting a probability model such as generalized Pareto distribution to the tail part. Reliability calculations are carried out using the limit state functions at the tail part. The reliability estimation is highly affected by the chosen threshold value and the shape and scale parameters of the probability model. In this paper, a methodology for choosing the optimum threshold value and model parameters is being investigated along with the effect of coefficient of determination (R2) and coefficient of variation of limit state functions. Mathematical example problems and a conceptual design of supersonic business jet aircraft are used as demonstration problems.

Probabilistic Optimization of a Stiffened Fuselage Panel under Fracture Constraints

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Stiffened fuselage panels are used as aircraft structural elements to carry combined loading. Stiffeners are used especially at the wing and the fuselage panels and exposed to the inner and the outer loadings. In this study, displacement compatibility method developed by Swift (1984) is used to perform fracture analysis of a stiffened fuselage panel. On the wide-bodied aircraft, fracture analysis of a two-bay cracked panel with broken central stiffener is examined under existing loadings. In order to illustrate the usefulness of the displacement compatibility method, a parametric study has been performed similar to a study that may take place during the development of any commercial aircraft structure. The example chosen is a two bay crack panel with a broken central stiffener that may be representative of a circumferential crack in the crown of a fuselage shell subjected to axial stress resulting from pressure and fuselage bending stresses. This parametric study indicated that three variables have the most influential effect on the geometry factor. These factors are the panel thickness, stiffener area and the stiffener spacing. Finally the panel thickness and stiffener area are optimized using probabilistic methods.

Void Coalescence under Combined Tension and Shear

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Most of the void coalescence models in the literature take only normal loads into account while neglecting shear loads, which can have an important effect on the coalescence process depending on the relative positions of voids and on the loading conditions. Shear loads can affect both the stress/strain at the onset of coalescence and the direction of deformation localization. Recently, a micromechanics based model is developed [1] by incorporating the effect of shear into the original void coalescence criterion of Thomason. In the mentioned study [1], the sole purpose was to determine the plastic limit load that initiates void coalescence; the void growth phase was out of scope. In this study, however, the effects of the void growth phase on coalescence under combined shear and tension will be investigated through FE analyses on 3D cuboid unit cells. The final goal is to build a micromechanics based void coalescence criterion that accounts for shape change and rotation of voids as well as the effects of shear loads.

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Selective Plasma Damage for Obtaining Free One Dimensional Nanoparticles

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One-dimensional (1D) nanostructures are of great interest in both fundamental and applied sciences due to their unique thermal, electrical, mechanical, and optical properties[1]. Among these particles, silica nano test tubes are novel inorganic nanostructures with several biotechnological applications including biosensing, magnetic resonance imaging, and targeted cancer therapeutics. They are generally prepared by sol–gel deposition of silica to nanoporous alumina templates[1]. Preparing samples composed of isolated free silica nano test tubes can be a challenging process due to the conformal coating of silica on the template. This causes the formation of a top-surface silica layer which laterally connects the nano test tubes (Figure 1) . Herein, we detailed the use of physical Ar^+ plasma etching to selectively remove this top-surface silica layer which yields free silica nano test tubes with template dissolution. Compared with the mechanical polishing approach, the plasma treatment allows a fine manipulation ability of the surface material at the nanoscale level. When used excessively, plasma etching causes an orifice closing phenomenon that can be explained with surface diffusion or viscous surface layer models.

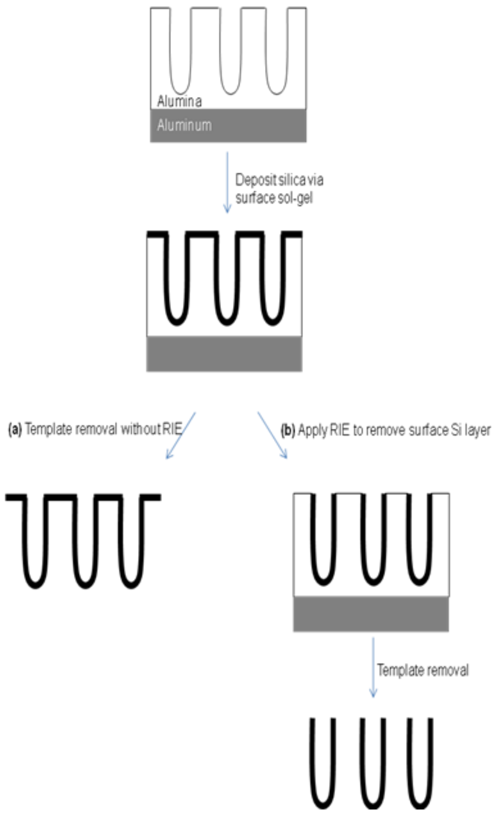

Figure 1. The rationale for using physical plasma etching for selective removal of amorphous silica

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Experimental Modal Analysis of a Pressurized Composite Tube with Cracks

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Keywords: plain weave, pressure vessel, crack, free vibration

Plain weave composite pressure vessels are increasingly preferred in many engineering areas [1]. Due to the complex performance against damage, both deformation and crack behaviors of such that type structures are to be well understood under different pressure conditions. In this study, dynamic analysis of aramid fiber plain weave pressure vessel with surface cracks subjected to different pressures is considered. For this purpose, vibration tests are performed to present the free vibration characteristics of clamped-clamped aramid fiber plain weave pressure vessel provided by TAI-Turkish Aerospace Industry Inc. Corresponding to the applied pressure, experimental dynamic analyses consist of three parts: (I) Vibration analysis with no-crack, (II) Vibration analysis with a surface crack, (III) Vibration analysis with two surface cracks. An impact hammer with a force transducer is used to excite the uncracked or cracked composite tube through the selected points. After the excitation, the responses are obtained by an accelerometer. The vibration measurements are completed using a microprocessor-based data acquisition system and nCode GlyphWorks software. Effects of crack type, size and location on the vibration characteristics are also examined experimentally.

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Abstract

This report covers the book of abstracts of the 2nd International Workshop on Physics Based Modelling of Material Properties and Experimental Observations, with special focus on Fracture and Damage Mechanics. The workshop is organized in the context of European Commission's Enlargement and Integration Action, by the Joint Research Centre in collaboration with the TOBB University of Economics and Technology (TOBB ETU) on 15th-17th May 2013 in Antalya, Turkey.
The abstracts of the keynote lectures and all the technical presentations are included in the book.
This workshop will give an overview of different physics-based models for fracture and degradation of metallic materials and how they can be used for improved understanding and more reliable predictions. Models of interest include cohesive zones to simulate fracture processes, ductile-brittle transition for ferritic steels, ductile fracture mechanisms such as void growth or localized shear, fatigue crack initiation and short crack growth, environmental assisted cracking. Experimental studies that support such models and case studies that illustrate their use are also within the scope. The workshop is also an opportunity for scientists and engineers from EU Member States and target countries to discuss research activities that could be a basis for future collaborations.

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