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Deutsche Gesellschaft für Materialkunde e.V.

Einladung zur Sitzung des Arbeitskreises Mikrostrukturmechanik im Fachausschuss Computersimulation der DGM

Die Frühlingssitzung des Arbeitskreises wird am

02. Mai 2018 ab 11:00 Uhr

im Hörsaal des Helmholtz-Zentrum Geesthacht stattfinden.

Die Adresse lautet **Max-Planck-Straße 1** in **21502 Geesthacht**.

Das Leitthema der Sitzung lautet

„Skalenübergänge in der Simulation heterogener Gefüge und Strukturen".

Wir laden Sie herzlich ein, an der Sitzung teilzunehmen und freuen uns auf ein interessantes und spannendes Treffen mit regen Diskussionen.

Mit freundlichen Grüßen,

Dr. Ingo Scheider, Helmholtz-Zentrum Geesthacht
Prof. S. Schmauder, Universität Stuttgart

Helmholtz-Zentrum Geesthacht
Centre for Materials and Coastal Research

Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre

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Programm:

11:00 – 11:15	Begrüßung *I. Scheider, S. Schmauder*
11:15 – 11:45	Influence of graphite morphology on static and cyclic strength of ferritic nodular cast iron using representative volume elements *Christian Gebhardt, IWM, RWTH Aachen*
11:45 – 12:15	A scale-bridging study on Damage evolution through cutting process for two different DP1000 steel sheets *Niloufar Habibi, IEHK, RWTH Aachen*
12:15 – 12:45	Comparison of the interaction behaviour of edge and screw dislocations with respect to precipitate interfaces *Dennis Rapp, IMWF, Uni Stuttgart*
12:45 – 13:45	Mittagspause
13:45 – 14:15	A Plasticity and Fracture Modeling Scheme on Multi-level Microstructure for Martensitic Steels *Peerapon Wechsuwanmanee, IEHK, RWTH Aachen*
14:15 – 14:45	Mehrskalensimulation der Verformung von Aluminiumschäumen *Martin Bäker, TU Braunschweig*
14:45 – 15:15	Highly parallel Molecular dynamics-Monte Carlo coupling towards solute segregation modelling *Hariprasath Ganesan, Institut für Werkstoffforschung, HZG*
15:15 – 15:30	Kaffeepause
15:30 – 16:00	Prediction of lamellar thickness dependent yield stress of PST-TiAl alloys using a mechanistic strain gradient crystal plasticity (MSG-CP) model *Rizviul M. Kabir, DLR Köln*
16:00 – 16:30	Separating the Hall-Petch strengthening effect of different coexisting microstructural boundaries in fully lamellar TiAl *Jan Schnabel, Institut für Werkstoffforschung, HZG*
16:30 – 17:00	Nonlocal modelling of deformation and damage behaviour of an inhomogeneous interphase in nano-particle supercrystals *Ingo Scheider, Institut für Werkstoffforschung, HZG*
17:00 – 17:15	Abschlussdiskussion *I. Scheider, S. Schmauder*

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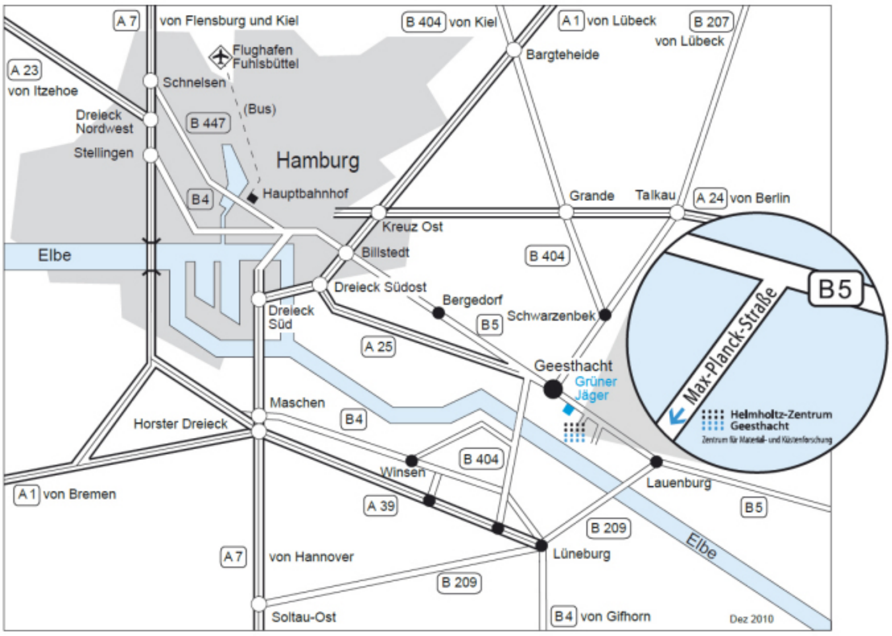
Venue's map:



More information about how to get to the HZG, please visit
https://www.hzg.de/about_us/visit_us/lageplan/geesthacht/index.php.en

Arriving by airplane:

Flights are available from Eurowings from Stuttgart and Köln/Bonn, arriving at Hamburg airport at 9:45h. We will provide a shuttle service picking up participants arriving by this connection.

Hotel recommendation

Hotel Lindenhof
Johannes-Ritter-Straße 38, 21502 Geesthacht
Telefon: 04152 84670

Hotel Elbblick
Elbuferstraße 102, 21502 Geesthacht (OT Grünhof-Tesperhude)
Telefon: 04152 2835

Influence of graphite morphology on static and cyclic strength of ferritic nodular cast iron using representative volume elements

Christian Gebhardt, Christoph Broeckmann, Alexander Bezold

Abstract

High silicon alloyed nodular cast iron consists mainly of a purely ferritic matrix and graphite nodules. Varying wall thicknesses and manufacturing conditions result in different graphite morphologies throughout a structural component. In this work, the microstructure is considered geometrically using a finite element (FE) approach with representative volume elements (RVE). The RVE models are derived from micrographs of fatigue specimen. The generated RVEs determine effective material properties through elasto-plastic homogenization and are subsequently analysed using a shakedown approach. In shakedown theory, the material re-enters the elastic regime after a few cycles of initial plastic deformation. This work uses melans theorem to derive a lower bound estimation of the endurance limit from a non-incremental calculation. Here, the material is modelled elastic-perfectly plastic. The major challenge in modelling nodular cast iron breaks down to the choice of suitable material constants for the graphite and ferrite phase, revealed by parameter studies on the static and cyclic model. Assuming reasonable material constants, fundamental effects, observed in the fatigue tests, were reproduced on the model level.

A scale-bridging study on Damage evolution through cutting process for two different DP1000 steel sheets

N. Habibi, V. Brinnel, S. Münstermann
Steel institute, RWTH Aachen University, Aachen, Germany

Abstract

The failure behavior of two different dual phase steel sheets, CR590Y980T-DP and CR700Y980T-DP, are compared. According to their ultimate tensile strength they are both categorized as DP1000, however they are slightly different from chemical composition and microstructural characteristics in terms of phase fraction and grain size. These differences result in considerable deviation in their damage behaviors. To reveal that, various testing methods along with digital image correlation (DIC) technique are employed. Therefore, the local strain changes can be detected for a wide range of stress-state. The results show that CR590Y980T-DP shows comparatively lower yield stress and higher hardening but fails without any significant localization. In the other hand, CR700Y980T-DP experiences considerable deformation after the damage initiates. Moreover, the damage behavior of the materials are modeled using the Modified-Bai-Wierzbicki damage criterion. This uncoupled damage model is able to predict damage initiation, damage propagation, and fracture. The calibrated damage models are employed to study materials' response through cutting processes. As the damage criterion is a phenomenological model, a virtual experiment model is also applied to take microstructural effects through the failure into consideration. In this regard, 3D representative volume element (RVE) models are created.

Keywords: Dual-phase steel sheets, Damage evolution, 3D Representative volume element, Cutting process

Comparison of the interaction behaviour of edge and screw dislocations with respect to precipitate interfaces

D. Rapp, S. Hocker, H. Lipp, S. Schmauder
University of Stuttgart

Abstract

Using molecular dynamics (MD) shear simulations, the interaction between dislocations of edge and screw type with precipitates were investigated within the material systems Ag-Cu and Cu-Ni-Si. For the former system, the investigated interfaces where incoherent, pointing particular interest to the dislocation reactions occurring at the Ag-Cu-interfaces due to the presence of misfit dislocations. For edge dislocations in the system Ag-Cu it could be shown that the regular interfaces of octahedral Ag-precipitates in Cu lead to cutting. However, spherical precipitates induce Orowan circumvention which is facilitated by the formation of Hirth locks due to reactions with full dislocations present at the precipitate interface, that prevent the trailing part of the incoming partial dislocation pair from entering into the precipitate [1]. On the contrary, screw dislocations with their ability to easily cross-slip have been found to completely circumvent the precipitate, i.e. the neither leave an Orowan loop behind nor cut through the precipitate for both spherical and octahedral shape.

For the Cu-Ni-Si system two coherent precipitate types were investigated: the cylindrical δ-Ni2Si precipitate and the spherical β–Ni3Si precipitate. To investigate this system via MD, an interatomic potential had to be developed for this material system [2]. It was found that edge dislocations cut through the spherical β-precipitates and Orowan circumvention only occurs in the case of high coherency strains. For the δ-precipitates, six different orientations relative to the Cu-matrix were investigated, of which only one was found to favour cutting. Screw dislocations were again found to circumvent the precipitates completely due to their tendency to cross-slip.

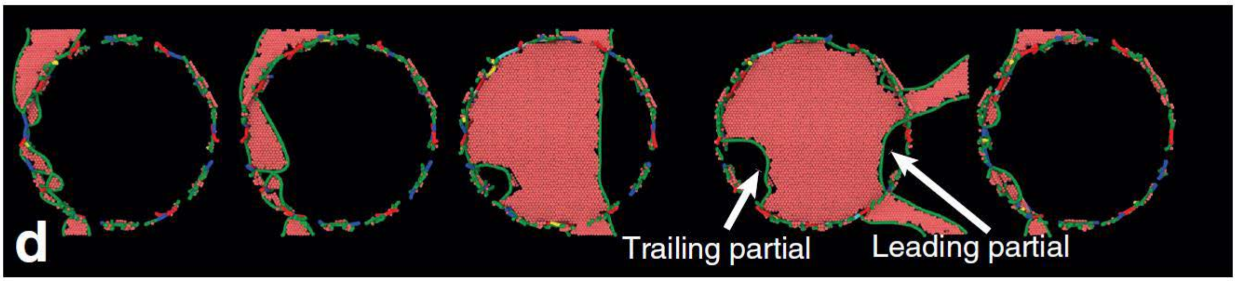


Figure 1: Cutting sequence of a spherical Ag precipitate in fcc-Cu by an edge dislocation that has dissociated in two partial dislocations. Shown in red are atoms in an hcp-configuration, i.e. stacking faults. Dislocation line segments are colored according to their type determined by DXA in OVITO, where blue segments represent full dislocations, green partials, yellow Hirth-locks, grey Lomer-Cottrell segments and red unnamed dislocation types.

References

[1] S. Hocker, D. Rapp, S. Schmauder Phys. Status Solidi B 254 (2017) 1600479.

[2] S. Hocker, H. Lipp, E. Eisfeld, S. Schmauder, J. Roth J. Chem. Phys. (2018) submitted.

A Plasticity and Fracture Modeling Scheme on Multi-level Microstructure for Martensitic Steels

P. Wechsuwanmanee, Z. Li, J. Lian, S. Münstermann
RWTH Aachen University, Aachen, Germany

Abstract

Martensitic steels have been widely used in many applications including agricultural machines, hopper ships, dredging lines, etc. due to its extraordinary strength compared to other steels. Despite its prevalence, its mechanical behaviors in terms of plasticity, damage or fracture have been sparsely revealed. The recent development on the extension of the modified Bai-Wierzbicki (eMBW) macroscopic model allows us to precisely describe the plasticity, damage and fracture characteristics independently from its microstructure features. This work proposes a multiscale modeling scheme, which does not only describe the plasticity behavior in the microscopic scale but also transfers the microstructure information to the macroscopic scale. Due to the unique multi-level microstructure of martensitic steels, a multi-level tessellation is applied to generating the artificial representative volume element (RVE) models. The generated RVE is then used for crystal plasticity constitutive model calibration by means of crystal plasticity finite element method (CPFEM). The model shall be validated by in-situ bending test with digital image correlation method. The scale-bridging approach is employed to link between macroscopic level and microscopic level to complete the description on plasticity as well as fracture.

Mehrskalensimulation der Verformung von Aluminiumschäumen

M. Bäker, J. Rösler, J . Tychsen, F. Haase, C. Teichmann

Abstract

Offenporige Aluminiumschäume können eingesetzt werden, um Lärm an Tragflügelhinterkanten zu reduzieren. Dabei ist die Porenform von besonderer Bedeutung, weil sie die Lärmentstehung beeinflusst. Eine Veränderung der Porenform lässt sich erreichen, wenn Aluminiumbleche gewalzt werden. Um diesen Prozess vorhersagen zu können, werden Simulationen auf mehreren Längenskalen Durchgeführt: Mesomechanische Simulationen dienen zur Bestimmung der genauen Materialeigenschaften auf deren Basis dann ein Kontinuumsmodell des Aluminiumschaums erstellt wird, mit dem der Walzprozess simuliert werden kann.

Prediction of lamellar thickness dependent yield stress of PST-TiAl alloys using a mechanistic strain gradient crystal plasticity (MSG-CP) model

Mohammad Rizviul Kabir, Mubeen Shahid
Institute of Materials Research, German Aerospace Center, Linder Höhe, 51147-Cologne

Abstract:

Lamellar spacing in multi-phase TiAl alloys influences the elastic, plastic, and creep behavior. A better understanding of these influences with respect to lamellar spacing can be obtained from the analysis of PST-TiAl alloy that consists of two-phase ($\alpha2+\gamma$)-TiAl lamellar structure. Many studies showed a distinct variation of yield stresses due to the thickness variation of the lamellar structure, and this phenomenon has been understood as “size-effects”. The commonly used classical crystal plasticity model (CPFEM) does not capture any size-effect; thus, they are not sensitive to the microstructural variation. In the present work, the size-effects in terms of local plasticity and yield for variable lamellae thickness has been captured using a strain gradient crystal plasticity (MSG-CP), which has been implemented in a classical CPFEM framework. In this approach, an intrinsic (material) length scale in the crystal plasticity constitute behavior has been introduced, as derived from the Tailor dislocation model. The model is able to predict local plasticity and global Hall-Petch effects as a contribution of statistically stored and geometrically necessary dislocations in the lamellar structures. The model seems promising to predict the size-dependency of the lamellar hardening; however, some discussion requires interpreting the model parameters with respect to the presented results.

Separating the Hall-Petch strengthening effect of different coexisting microstructural boundaries in fully lamellar TiAl

Jan Eike Schnabel[1], Swantje Bargmann[2]
[1] Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Germany
[2] Chair of Solid Mechanics, University of Wuppertal, Germany

Abstract:

In this article, we present a strategy to decouple the relative influences of colony, domain and lamella boundary strengthening in fully lamellar titanium aluminide alloys, using a physics-based crystal plasticity modeling strategy. While lamella and domain boundary strengthening can be isolated in experiments using polysynthetically twinned crystals or mircomechanical testing, colony boundary strengthening can only be investigated in specimens in which all three strengthening mechanisms act simultaneously. Thus, isolating the colony boundary strengthening Hall-Petch coefficient K_C experimentally requires a sufficient number of specimens with different colony sizes λ_C but constant lamella thickness λ_L and domain size λ_D, difficult to produce even with sophisticated alloying techniques. The presented crystal plasticity model enables identification of the colony boundary strengthening coefficient K_C as a function of lamella thickness λ_L. The constitutive description is based on the model of a polysynthetically twinned crystal which is adopted to a representative volume element of a fully lamellar microstructure. In order to capture the micro yield and subsequent micro hardening in weakly oriented colonies prior to macroscopic yield, the hardening relations of the adopted model are revised and calibrated against experiments with polysynthetically twinned crystals for plastic strains up to 15%.

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Nonlocal modeling of deformation and damage behavior of an inhomogeneous interphase in nano-particle supercrystals

Songyun Ma, Ingo Scheider, Swantje Bargmann
Institute for Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht

Abstract:

A novel nano-particle composite synthesized by bio-inspired design has been fabricated, which shows extraordinary mechanical characteristics due to the well-organized arrangement of soft and hard constituents in the microstructure. For this material, the inhomogeneous interphases surrounding the nano-particles play an important role in the mechanical performance of nano-composite.

In order to describe this material on the nano-scale, particularly the interphase region, a nonlocal material model based on micropolar theory is proposed. The new model is able to account for the scale of microstructure and describe the inelastic behavior, namely damage and plasticity, of interphases with gradient material properties. Micromechanical simulations are performed to investigate the relationship between nanostructures and mechanical properties of nanocomposites. The proposed damage model is validated by 3D micromechanical simulations for the nanoparticle super-crystals fabricated at different temperatures. The simulation results are in good agreement with the experimental data from micro-cantilever beams in terms of the stiffness, tensile strength and fracture energy absorption of the nanocomposites.

References

[1] S. Ma, I. Scheider, S. Bargmann: Ultrastrong nanocomposites with interphases: nonlocal deformation and damage behavior, submitted to *Mech. of Mater.*