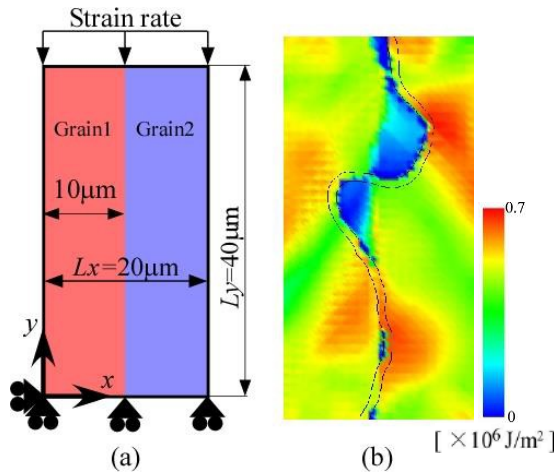


Development of Multi-phase-field Crystal Plasticity Model for Grain Boundary Bulging during Dynamic Recrystallization

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In hot working of metal material with low to medium stacking fault energy, microstructures are refined due to dynamic recrystallization (DRX). During the DRX, grain boundary bulging serves as a major nucleation origin of DRX grains [1]. Therefore, in order to accurately predict the nucleation site of DRX grains, it is important to understand the nucleation mechanism of DRX grain by grain boundary bulging. For that purpose, it is essential to develop a numerical model for DRX. However, because DRX is a highly complicated phenomenon where grain growth and plastic deformation occur simultaneously, to our knowledge, models that can express the grain boundary bulging have not been reported so far.



In this study, we develop a DRX model by coupling crystal plasticity (CP) model and multi-phase-field (MPF) model [2] to make clear the DRX nucleation mechanism due to grain boundary bulging numerically. In this model, non-uniform deformation, dislocation density and crystal orientation of poly crystalline structure are computed by CP finite element method. At the same time, MPF simulation is performed to express grain growth driven by stored energy of dislocations and redistribution of dislocation density due to the grain boundary migration. Dislocation densities and crystal orientations are exchanged between these two computations.

Figure 1: (a) Computational condition for compression simulation of bi-crystal material. (b) Grain boundary and stored energy distribution at 32% compression.

Fig.1 (a) shows the computational condition for compression simulation of bi-crystal material with different crystal orientations. Fig.1 (b) shows the calculation result of MPF simulation at 32% compression. Color and solid line indicate stored energy distribution and grain boundary, respectively. It is observed that the grain boundary migrate to the area with high stored energy and the stored energies behind the migrated grain boundary become small. From this result, it is confirmed that the developed model can express grain boundary bulging during DRX well.

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Analytical method for estimating the thermal expansion coefficient at high temperature

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Recent years, the development of materials for high temperature environments, in the field of the high-efficiency thermal power plant has become active. Since try-and-error scheme has reached the limitation, the estimation of physical properties by atomic-scale simulation is desired. In estimating of the thermal properties at high temperature, thermal expansion coefficient is one of key material property. It is said that the thermal expansion of the crystal is caused by the anharmonicity of the lattice vibrations. Conventional method based on the quasi-harmonic approximation [1] is known that the accuracy decreases at high temperature because the model does not sufficiently include the effect of the anharmonic vibrations [2].

In this study, we proposed an analytical method for calculating the thermal expansion coefficient at high temperature by estimating the distribution of interatomic distances based on the phonon-dispersion relation. The model incorporates the anharmonic effect caused by the increase in the amplitude of the phonons.

Classically, the pressure can be calculated by the interatomic potential and the radial distribution function using the Virial equation. Therefore, assuming the harmonic approximation, we estimated the radial distribution function from the relationship between the energy and the amplitude of the phonons. We take into account several anharmonic effects, such as the variation in the frequency of the phonons, the increase in

the distance between atoms due to the vibration, the asymmetry of the interatomic potential. By considering these effects quantitatively, our proposed model allows us to estimate the thermal expansion coefficient analytically over a wide temperature range.

Development of the interatomic potential which reproduces the thermal expansion coefficient at high temperature has become possible. We have developed the interatomic potentials for Ni and Fe to reproduce the thermal expansion coefficients over a wide temperature range.

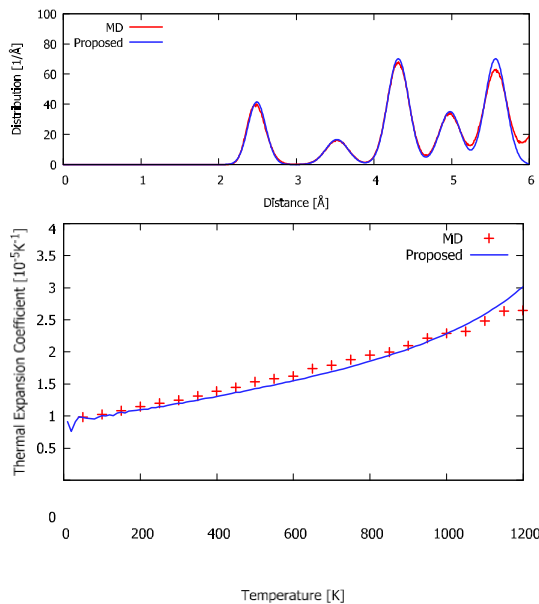


Figure 1: Estimation of radial distribution function (upper) and thermal expansion coefficients (lower) of Nickel.

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Dynamic Recrystallization Modeling by Multi-phase-field Method Considering Misorientation Dependent Interface Properties

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Dynamic recrystallization (DRX) occurs during hot-working of metallic materials with low to medium stacking fault energy. Macroscopic mechanical behaviors during the hot-working with DRX are largely affected by the microstructure evolutions, or DRX grain growth. Therefore, in order to estimate and predict hot-working properties with high accuracy, it is key to develop a multi-scale model for DRX, which can compute the macroscopic mechanical behaviors depending on the microstructure evolutions.

We have developed a multi-phase-field dynamic recrystallization (MPF-DRX) model [1-3], where the evolution of dislocation density, or plastic deformation, is modeled by the Kocks-Mecking model and DRX grain growth is simulated by a multi-phase-field (MPF) method. Average stress of the computational domain is computed by Bailey-Hirsch equation using the average dislocation density of the domain. This MPF-DRX model enabled us to compute the mechanical behaviors of the domain based on the DRX grain growth, or multi-scale simulation of hot-working with DRX. On the other hand, the MPF-DRX model assumed that the dislocation density is constant in a grain and the grain boundary energy and mobility are constant independent on the grain boundary misorientation. In order to perform more accurate evaluations of hot-working, the model needs some improvements.

In this study, we develop the modified MPF-DRX model by introducing misorientation dependencies of grain boundary energy and mobility to the MPF model and a preferred nucleation site. The MPF model used in the present MPF-DRX model, which was developed by Steinbach et. al. [4], is difficult to introduce grain boundary energies and mobility with large difference. To improve the point, we introduce novel way to accurately express the grain boundary properties at triple points. In addition, the information of preferred nucleation site, such as triple point, grain boundary and inside of grain, is introduced to the MPF-DRX model. By performing a series of simulations using the modified MPF-DRX model, we confirm the accuracy of the model and the effects of the modified points on the results. In addition, the modified MPF-DRX model is incorporated to the MPFFE-DRX simulation [5] and we try to simulate more realistic hot-working multi-scale simulations.

This work was supported by JSPS KAKENHI Grant Number 25630011.

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Computational model verification using multiplexed photonic Doppler velocimetry for high velocity projectile impact on steel targets

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Metal plates are subjected to high stress and strain rate deformation in penetration experiments and results are modeled using two complementary approaches. This work presents a unique approach to experimentally measuring the velocity of the back surface of the target at several points during the early deformation phase. Crater details are measured after the impact and all measurements are compared to computational simulations.

A two-stage light gas gun was used to launch cylindrical Lexan projectiles at velocities from 4 to 6 km/s at a 12.7 mm (0.5") thick ASTM A36 steel plate. The impact creates a small crater in the front of the plate and a bulge on the back surface, which typically leads

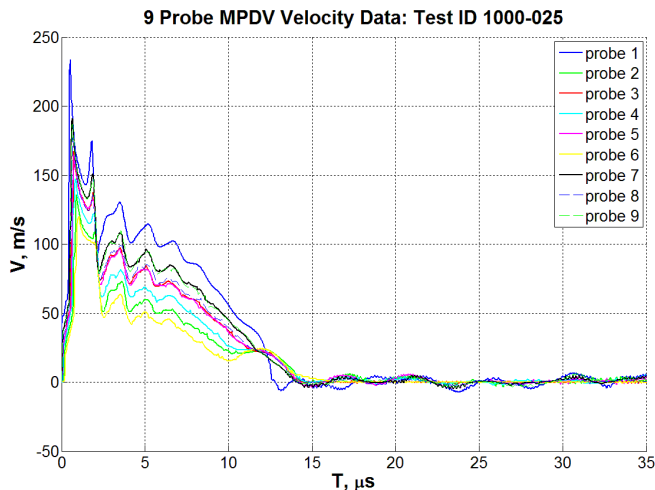


Figure 1: Sample data from a penetration experiment

to fracture and spallation of material near the back face. The free surface velocities from multiple points on the plate's back surface are measured using a Multiplexed Photonic Doppler Velocimetry (MPDV) diagnostic system. PDV is an interferometric fiber-optic technique that can determine velocity by measuring the Doppler shift of light reflected from the moving surface.

The Lagrangian-based smooth particle hydrodynamics approach in LS-DYNA and the Eulerian-based CTH hydrocode are used to simulate all experiments. Both models use a combination of the Johnson-Cook material model and the Mie-

Grüneisen equation of state. Experimental data and simulation results are compared to verify the accuracy of the computational models during ballistic impact events.

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A multiphase-field model with Onsager reciprocal relations

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A generalization of the multiphase-field model [Steinbach I. and Pezzolla F.; *Physica D* 1999;134;385] to include kinetic cross coupling to a conserved field [Brenner E.A. and Boussinot G.; *Phys Rev E* 2012;86;060601] is presented. We show that this model is consistent with phenomenological relationships given by Onsager and his predecessors including symmetric reciprocal relations having a positive-definitive matrix of kinetic parameters (positive entropy production). At junctions, the interaction between each phase-field is attributed by a coupling term to all other existing phase-fields and the respective conserved order parameters. The model shall be applicable to phase transformations with kinetic constraints on the transformation rate at dual interfaces and junctions between an arbitrary numbers of fields.

Modelling nonlinear behavior of heterogeneous geomaterials by extended finite-element method

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Predicting the behavior of heterogeneous materials has attracted the attention of the research community mainly because they are used in various engineering applications coupled with more restrictive safety rules. However, both for natural and industrial materials, accurate behavior modeling is still a challenge despite of the fast progress of modeling techniques because of the need for a more precise knowledge of the mechanical properties for the structural behavior. Moreover, geomaterials like rocks or soils used for the nuclear waste disposal are known to have a non linear behavior and are particular class of heterogeneous material strongly influenced by their geological history and their natural composition and requires considerable efforts. To describe the mechanical behavior of such material, two approaches have been proposed. The macroscopic one suppose the material homogeneous, have the same behavior at any point , and use a well-established plastic viscoplastic and damage models identified by laboratory tests. The micromechanical approach complements the first by considering the microstructure of the material and the behavior of each constituent by highlighting the role of the microstructure and the interaction of their mechanisms on the macroscopic behavior. In spite progresses of numerical upscaling approach with complex behavior, the microstructure is simplified and described the well known unit cell. Alternatively to classic finite element method, XFEM offers to homogenization method the possibility to describe a more complex microstructure [1].

The M-H-M argillite rock studied in this work shows macroscopic nonlinear strains caused by slip of clay sheets of argillaceous matrix, and the damage of the matrix or grains [2]. In this paper, we are interested in modeling the behavior of the argillite rocks by numerical homogenization based on XFEM (extended finite element method). To describe the nonlinear behavior of the constituent the associated Drucker-Prager model is integrated in the XFEM computer code developed with Matlab [3]. The material is considered as biphase composite with elastoplastic matrix and elastic inclusions and pores with different shape and spatial distributions.

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Crack Propagation Simulations in Polycrystal by Multi-phase-field-crack Model

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Crack propagation problem is the important and difficult point of study among the fracture mechanics. In particular, a prediction of crack propagation path in a complicated microstructure is very difficult. In numerical prediction and estimation, finite element methods are widely used to simulate the crack propagation. Meanwhile, finite element method needs to track the crack tip position and to select a direction of crack propagation. Therefore, it is thought to be difficult to simulate crack propagation in complicated microstructure only by finite element method.

Recently, studies where a phase-field method is applied to the prediction of crack propagation are done actively [1]. In phase-field method, crack and material is distinguished by an order parameter, or phase-field variable, and the crack interface is expressed as a variation region of the phase-field. The merits of the phase-field method are that we do not need to track the crack tip and that the crack propagation direction is determined automatically. Therefore, the phase-field method is promising method in the problem of crack propagation prediction.

In this study, we have developed multi-phase-field-crack (MPFC) model which can predict crack propagation in complicated microstructure of brittle material. In this model, we use the multi-phase-field model proposed by Steinbach et. al. [2] for grain growth and polycrystalline phase transformation. Elastic anisotropy, crystal orientation, difference of fracture toughness inside grain and at grain boundary, and misorientation dependent grain boundary energy are introduced into the MPFC model. By simulating crack propagation in polycrystal using the developed MPFC model, we confirm the validity of the developed model.

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Impact of extended defects on the mobility of grain boundaries: A molecular dynamics study

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Classical molecular dynamics simulations are commonly used to explore the migration of grain boundaries. Our previous research has shown that conclusions drawn from such studies are highly dependent on systems size and driving force [1]. In particular the concept of an intrinsic mobility must be abandoned for perfectly flat, symmetric grain boundaries below the roughening temperature.

The present study extends our research towards grain boundaries deviated from their perfect and symmetric arrangement. Such boundaries constitute in fact the majority of experimentally observed moving boundaries. We introduce defects of different configurations into several low sigma high angle grain boundaries through systematically inclining the boundary plane from a symmetric equilibrium boundary. The results of the simulations show how the mobility of a boundary increases as the level of planar asymmetry increases. The results further show that the propagation of steps (which asymmetric boundaries relax into) is the rate determining mechanism of migration of the studied grain boundaries.

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On the strength properties of ductile porous solids with a Mohr-Coulomb matrix: theoretical formulation and numerical assessment

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We propose a new analytical macroscopic strength criterion for porous solids having a rigid-perfectly plastic matrix obeying Mohr-Coulomb yield criterion. In the context of a standard limit analysis, an associated flow rule is considered. We derive in a parametric form a closed-form expression of the macroscopic criterion. To this end, and similarly to the pioneering study by Gurson [1] (for von Mises matrix) and Guo et al. [2] (for a Drucker-Prager matrix), we perform a kinematic limit analysis homogenization of a hollow sphere under axisymmetric loadings. In the present study, a minimization problem, arising in the determination of the macroscopic plastic dissipation potential, has been solved analytically by means of Lagrangian methods of inequality constrained optimization. The predictive capabilities of the derived strength criterion are successfully assessed by comparison with numerical limit analysis results delivering lower and upper bounds of the macroscopic criterion of the porous solids with a Mohr-Coulomb matrix [3,4]. The influence of the third stress deviator invariant on the macroscopic strength surface is also highlighted through the asymmetry of the macroscopic yield surface with respect to pure hydrostatic axis. Moreover, it is shown that the tension-compression asymmetry of the Mohr-Coulomb yield surface at micro-scale, with respect to the pure deviatoric axis, is transposed at macro-scale by the homogenization procedure.

This work was performed under the financial support of the program “Transports durables et mobilité” via the French project ANR CoMatCo.

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Diffusion of oxygen in TiNiHf high temperature shape memory alloy: A first-principles approach

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The need of high temperature shape memory alloys (HTSMA) is increasing due to their potential applications for various mechanical devices such as actuator in automobile engine. In order to increase the operating temperature of SMA, various alloy systems including NiTi-X (X = Pd, Pt, Au, Rh, Zr and Hf) have been examined extensively. In a point of view of a materials cost the Ni-Ti-Hf system is a one of promising candidates which exhibit high transformation temperature and superior shape memory characteristics. However, the Ni-Ti-Hf HTSMAs have not been commercially available yet due to processing difficulties such as control of chemicals and mechanical processing partially coming from oxidation, as with other TiNi based HTSMA systems.

The oxidation behavior of $\text{Ni}_{0.5}\text{Ti}_{0.5-x}\text{Hf}_x$ alloy should be examined carefully because annealing and fabrication temperature of this alloys are enough high to be readily oxidized. Recently, one of authors reported that the oxygen diffusion in $\text{Ni}_{0.5}\text{Ti}_{0.5-x}\text{Hf}_x$ alloy is much faster than that in NiTi based on isothermal oxidation experiment with a TGA, however, the effect of dopants on the oxygen diffusion was not fully understood [1]. Therefore further systematic investigations via both of experimental and theoretical methods are necessary to understand the oxidation behavior.

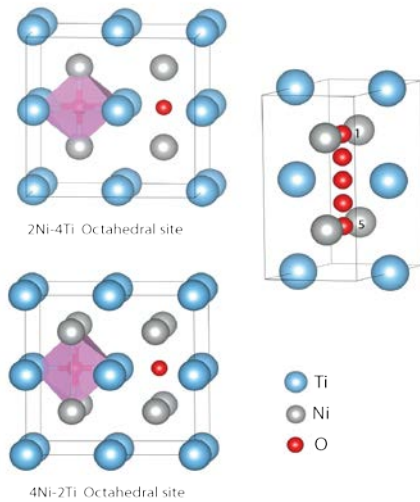


Figure 1: Two kinds of octahedral sites in NiTi and diffusion path

In this presentation, systematic nudged elastic band (NEB) calculations were performed with the VASP to obtain the activation energy of oxygen diffusions. In NiTi, there are two kinds of octahedral sites as shown in Fig. 1. It was found that the interstitial oxygen diffuses the neighbors with the lowest activation energy via two different octahedral sites and the activation energy is strongly related to the size of octahedral site. In order to understand the effect of dopant, a bigger calculation cell containing Hf atoms was carried out and the effect of structural relaxation around the defect was examined systematically. In addition, the effect of dopant concentration with special quasi random structures will be discussed.

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Phase transformations in Fe-C bulk and nanowire systems: molecular dynamics simulation and free-energy calculations

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Using molecular dynamics simulation, we study the austenite-martensite phase transition in the Fe-C bulk system for C contents up to 1 at% [1]. The systems are subjected to a heating/cooling cycle. The transition temperature can be determined from the hysteresis of the system volume with temperature. We observe that the martensite temperature decreases with C content, as in experiment. In the austenite phase we find strong twinning.

We supplement the studies with free-energy calculations based on both thermodynamic integration and perturbation theory [2]. The results agree well with our atomistic simulations.

We employ the Meyer-Entel potential for describing Fe-Fe interactions [3], while the pairwise potential by Johnson et al. [4] was used to model Fe-C. C-C interact by the Tersoff potential.

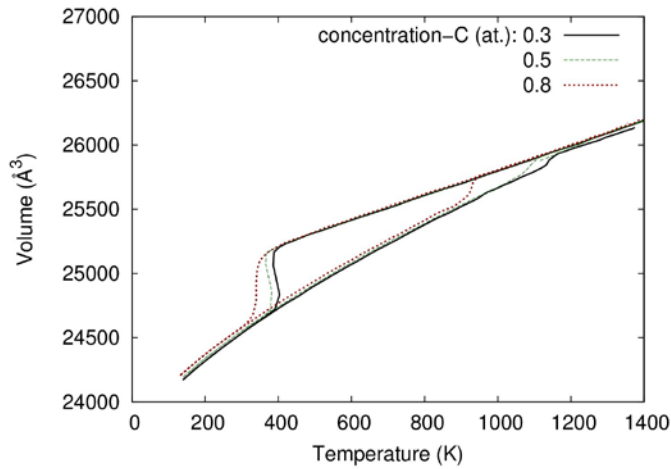


Figure 1: Dependence of the system volume on temperature during a heating / cooling cycle (bulk system). C concentrations are 0.3, 0.5, and 0.8 at %.

In addition, we study nanowire systems in order to assess the influence of free surfaces on the mechanism of transformation [5].

The bulk system follows the Nishiyama-Wassermann path, while the Kurdjumov-Sachs orientation relationship is fulfilled in the nanowire. Under axial stress in nanowires, the martensite transformation is partially suppressed, creating strong plastic deformation.

This work is carried out in the Collaborative Research Center CRC 926 “Microscale Morphology of Component Surfaces”. Funding by Deutsche Forschungsgemeinschaft is gratefully acknowledged.

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Principal component analysis of necking in sintered nanoparticles

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Sintering mechanism of nanoparticles have been a subject of wide interest owing to its role in the deciding their catalytic properties. Reduction of surface energy is believed to be the principal driving agent of nanosintering. Even though several attempts have been made to understand the underlying thermodynamics through modeling and atomistic simulations [1,2], expression of the kinetics remains a difficult problem. A major obstacle in this regard arises from the fact that the particles consist of thousands of atoms and the state of the system at any instant needs a very large number of variables to be expressed. Therefore, somewhat crude measurements like neck-width and radius of gyration are often used to specify the current state of the system.

In the present work, I propose the use of dimensionality reduction by means of principal component analysis [3] and employ the principal projection of atomic coordinates to express the instantaneous state of nanoparticles undergoing the process of sintering. Once the principal component of the atomic trajectories is obtained, other kinetic parameters, like the rate of sintering process, effective thermodynamic forces and the effective thermodynamic inertial are obtained easily. This technique has been applied for two cases: first, the sintering simulation is carried out under isothermal conditions and second, the sintering takes place under linearly rising temperature. The fundamental differences between these two modalities have been explained and they are analyzed from the perspective of their corresponding principal components.

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Reversible multiscale homogenization for obtaining effective strength-elastic properties of composite materials with incomplete set of initial data

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This work presents the continuation of series of research works about developing mathematical models of mechanical properties of composite materials [1,2] based on multiscale homogenization method or asymptotic averaging method (known under this name in Russian scientific journals). Like in previous works the effective strength-elastic properties of composites are the main objective, but the difference is that at it was made an attempt to handle the situation when the set of initial data is incomplete. New computational technique tries to estimate missing data first before making a decision of simplification the model of material of components of composite. New computational method and corresponding software implementation were built and some of its main features are presented here. This software was created to support the design process of new composite materials with predetermined properties. Expected that new computational method make it possible to increase the accuracy of final computed effective properties of modeled composite materials in comparison with experimental data in case when the set of initial data is incomplete (for example: strength-elastic properties of carbon fibers in transverse direction to the fiber axis are usually unknown). To find the solution of the problem in such case direct and inverse tasks of the mechanics of composites were solved together. All of these tasks were combined into the single network model of the whole task automatically by means of usage of developed software. New computational method was named Reversible multiscale homogenization (RMH). Some computational results are presented at Fig. 1.

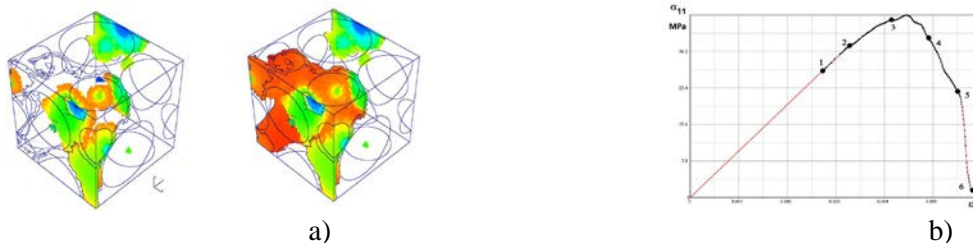


Figure 1: Computed Stress-strain diagram (a) of the model of unit cell of fiber-reinforced composite material (b). Destruction process simulation.

This work was performed with financial support from the Ministry of Education and Science of the Russian Federation (grant of President of Russian Federation MK-6573.2013.3 and State Order to Higher educational institutions □1.6260.2011).

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Bridging Crack Propagation at Atomistic and Mesoscopic Scale with Hybrid Multiscale Methods

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Modern methodology to the modeling and simulation of crack propagation uses cohesive finite element methods (FEM) based on some type of cohesive constitutive laws. Physically, these laws should be developed based on the data obtained from atomistic crack simulation following the fact that crack propagation originates from the atomistic scale. However, reports show that directly use the data from atomistic-based simulation for FEM and meso- and macroscopic analysis is not practical. In most cases, one needs to revise the data such as reducing the obtained traction stress greatly or using empirical traction-displacement law to make the simulation convergence towards the realistic experimental results. This large discrepancy between the method based on physics and the empirical practice has motivated the present work to see whether this is caused by the simulation method itself. To reach this good, we use a hybrid multiscale method which combines the concurrent generalized particle dynamics (GP) method proposed by Fan et al. since 2009^[1-4] and the bottom-up hierarchical method to transfer the GP-obtained physical parameters to the upper mesoscale FEM to investigate the meso- and microscopic crack propagation.

Here, the high-accuracy of atomistic crack simulation is essential and is warranted by the GP method. GP is one kind of coarse grain methods, but it has special features that the model consists of several particle domains of different scales with scale $n=1$ being atomistic scale and a large scale $n=2, \dots, m$ corresponds to continuum. The GP uniqueness include: First, the structure of all particle domains is the same as the atomistic domain and all calculations in the particle domain are conducted in its corresponding atomistic domain by the inversed mapping method. Second, the GP concept of scale duality can allow material being particles by a lumping process and being atoms when they are near, say, crack tips and interface by decomposition. This feature makes GP capable to extend MD models with sizes several orders larger than MD to raise its accuracy. To get detail physical data in terms of the crack propagation distance, Δa , from the tip O of pre-setting edge crack of length a , 20 rectangular rectangle atomistic subdomains I ($I=1, 2, \dots, 20$) are divided for the area in front of the origin crack tip O. The center coordinate of each generic subdomain is $X_I = I \cdot 20A$ where $20A$ is the width of the subdomain and its height is $80A$. We take the subdomain I as the fundamental material object to observe the material behavior against the crack propagation when the current crack tip propagates to the subdomain, i.e., when $\Delta a = X_I$. In this way, for each subdomain I ($I=1, \dots, 20$) three important physical variables are obtained: (1) The maximum resistance stress, $\sigma_{I-\max}$, of the material to against the crack passing through the subdomain I. (2) The rate of the resistance increase to reach $\sigma_{I-\max}$ measured by the initial slope of the stress-crack surface separation diagram (i.e., $\sigma_I \sim \delta$ curve). This parameter indicates the material hardening behavior to crack propagation. (3) The area under the $\sigma_I \sim \delta$ curve gives the energy release rate G_I which is an important energy variable for crack propagation. The GP results by drawing curves connected all the points of $\sigma_{I-\max}$ and G_I for all the 20 subdomain show interesting feature of the subdomain resistance. Inputting directly these GP-determined data sets for a cohesive finite element analysis of a compact fracture specimen, the critical force P as well as the critical stress intensity factor K_{IC} for the crack propagation is obtained. The result seems reasonable and encouraging. In the presentation, we will show more results in relation to using the hybrid method for the mixed mode loading, rate effects, and the FEM results from the data set at different subdomain as well as the discussion related to the common used cohesive constitutive law and methods.

Modeling of buckling under residual stresses by arlequin method and asymptotic numerical method: application to rolling of thin sheet metal

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In this paper we present a new numerical technique to model the buckling phenomena under residual stresses induced by rolling process. This technique consists in coupling two finite element models: the first one consists in a three dimensional model based on 8- node tri-linear hexahedron which is used to model the three dimensional behaviour of the sheet in the roll bite; the second model is based on a shell formulation well adapted to large displacements and rotations, it will be used to compute buckling of the strip out of the roll bite [1]. We propose to couple these two models by using Arlequin method [2]. The originality of the proposed algorithm is that in the context of Arlequin method, the coupling area varies during the rolling process. Furthermore we use the asymptotic numerical method to perform the buckling computations taking into account geometrical nonlinearities in the shell model [3]. This technique allows one to solve nonlinear problems using high order algorithms well adapted to problems in the presence of instabilities.

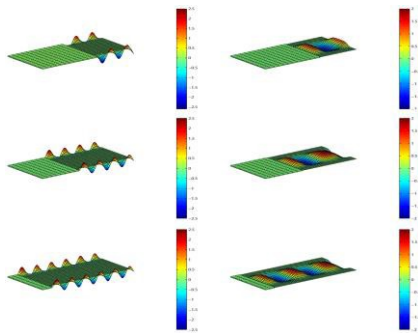


Figure 1: Propagation of the edge-waves flatness defects

The proposed algorithm is applied to some rolling cases where “edges-waves” and “center-waves” defects of the sheet are observed. The numerical results are compared with experimental data. To simulate the advance of the sheet in the process, the residual stress field is translated along the sheet. The position of the roll and the coupling area are located by a parameter which varies along the length of the sheet. The propagation of the edge-waves and the center-waves buckling are presented in the figure 1.

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