Abstracts

Peter M. Derlet NUM-Condensed Matter Theory Group Paul Scherrer Institut CH-5232, Switzerland	**Atomistic modelling of metals: Introduction and Applications** Atomistic simulation can provide kinetic and dynamical insight into the fundamental component processes underlying both mass-transport and plasticity within a solid. To directly extrapolate atomistic simulation results to the experimental time-scale is however difficult and remains a general challenge to the atomistic modelling community. This is particularly the case when performing simulations that investigate the plastic response of a material, where strain rates are generally 8-10 orders of magnitude faster than that seen in experiments. The present series of lectures gives an introduction to the basics of atomistic modelling methods and case-studies a number of examples that demonstrate both the power of the technique and its corresponding caveats. The first lecture will give an introduction to the atomistic method covering the molecular dynamics method, structural relaxation, reaction path calculation methods and semi-empirical potential development. The second lecture will give a number of atomistic simulation examples that exist in the published literature concentrating on point-like defects and their diffusion, and atomic scale plastic processes such as dislocations and their interaction with structural defects. How such information can be used in higher length- and time-scale modelling methods will also be addressed. In both lectures the time-scale problem inherent to the molecular dynamics technique will be discussed and the atomistic acceleration techniques that have attempted to overcome this will be reviewed.
Stefan Müller University Erlangen-Nürnberg, Lehrstuhl für Theoretische Physik 2 Staudtstr. 7 D-91058 Erlangen	**Computational materials science on an atomistic basis: A multi-scale problem** Although modern computer codes based on density functional theory (DFT) allow the reliable prediction of many material properties, they cannot be applied, when the problem of interest demands a consideration of huge configuration spaces or model systems containing many thousand atoms. Moreover, DFT based methods do not allow for exchange processes between atoms and therefore, do not consider configurational enthalpies being a prerequisite for modeling the temperature-dependence of substitutional ordering phenomena in multi-component systems.

	In principle, the combination of methods allowing for studying dynamic processes on the atomistic scale as molecular dynamics (MD) (introduced in this summerschool) with DFT would be a powerful tool to overcome these limitations, if we find a key to couple these individual approaches. It will be demonstrated that one very successful concept to “open the door” is the use of so-called Cluster Expansions (CE) and Monte-Carlo Simulations (MC). It will be shown, how these “multi-methods approach” of DFT, MD, CE, and MC permits us to treat material properties up to the mesoscale without any empirical parameters as input, but with an accuracy that allows the quantitative comparison with experimental results. The focus will be on processes which possess a delicate time- and temperature-dependence like short-range order or precipitate evolution.
Daniel Weygand izbs Universität Karlsruhe (TH) KIT Kaiserstr. 12 D76131 Karlsruhe, Germany	**Three dimensional discrete dislocation dynamics modelling: Introduction and Applications** The mechanical properties of crystalline materials are determined by the evolution of the dislocation microstructure within the sample. The dislocation motion in small structures is strongly determined by geometrical constraints and often a so called size effect in the flow stress ,“smaller is stronger”, is observed. Continuum modelling cannot easily capture size effects, as the characteristic length scale of the dislocation microstructure, e.g. the average spacing between dislocation, and the sample size are too close, and therefore averaging is not allowed. The method of „discrete dislocation dynamics“ (DDD) is able to handle this situation, as the motion of the dislocations is explicitly tracked. The first lecture will give an introduction to the physics of dislocations and their description within linear elasticity theory, needed for the formulation of a discrete dislocation dynamics model. The following points of the model will be detailed: • geometrical description of dislocation in a DDD model • basics of dislocation interactions and reactions • constitutive rules for dislocation motion • treatment of boundary conditions The second lecture focuses on applications of discrete dislocation modelling. The stability of specific elementary dislocation interactions will be discussed as well as the interaction of dislocation with

	obstacle fields both in comparison to MD simulation and to experimental studies. Furthermore the role of dislocation source activation will be discussed, to explain the flow stresses of observed in thin films. The last series of examples is inspired by numerous studies on the mechanical behaviour of micrometer-sized pillars, produced by FIB (Focused Ion Beam). The DDD method is applied to analyse the size dependency of the measured flow stresses including an analysis of the so-called “strain bursts”, which are a common feature of the stress strain curves. Simulated bending and torsion test are compared to experimental observations and the resulting dislocation microstructure is analysed to explain the observed behaviour.
Marc Fivel SIMaP CNRS/Grenoble Institute of Technology	**Dislocation dynamics simulations and scale transitions** Three lectures will be given in order to highlight the role played by discrete dislocation (DD) simulations in multi-scale modelling of crystal plasticity. DD simulations can indeed fill the gap between atomic simulations (molecular dynamics) and continuum modelling (finite element techniques). The first lecture will focus on molecular dynamics (MD) simulations dedicated to the study of dislocation behaviour. These simulations are needed to feed DD modelling when elasticity cannot predict some situations. It can be the case for thermally activated mobility of screw dislocations in bcc materials. It is also the case of irradiated materials where dislocations react with Frank loops. Another example concerns dislocation nucleation in confined plasticity like during indentation tests. For all these examples, dislocation reactions can be derived from MD simulations and introduced as local rules in DD codes. The second lecture will follow the two lectures given by Daniel Weygand who will present the details of DD modelling. We will focus on applications where dislocation dynamics simulations gave concrete results useful for engineering mechanics. Two examples will be presented. The first one deals with fatigue simulations of AISI 316L stainless steel. Simulations performed under various loading and boundary conditions show the crucial role played by cross-slip in the formation of the dislocation microstructure. As the cycling proceeds, slip bands exhibiting well organised dislocation arrangements progressively substitute to dislocation tangles. Calculations of the plastic steps printed on the free surface during the cycling give access to the surface relief which is found to be made of extrusion and intrusion profiles. Analyses of stress and distortion energy concentrations inside the slip bands reveals

	that a crack would most probably initiate at the surface when multipoles, driven by interfacial dislocations, will reach the surface. The second example concerns the simulation of nanoindentation tests. This simulation requires coupling DD with FEM in order to enforce the boundary conditions. A nucleation criterion is introduced based on MD simulations. The effect of cross-slip probability on the remaining dislocation microstructure after unloading is analyzed. Indentation size effect, which denotes the decrease of the hardness when the penetration depth in increased, is addressed. Surface relief are analyzed and compared to AFM observations. The last and third lecture will focus on the transition between DD simulations and continuum mechanics. A set of constitutive equations based on dislocation densities is presented. Each equation is demonstrated from the individual behaviour of dislocation motion in a glide system. Since these equations are based on a physical description of dislocation plasticity, the involved parameters can be identified using DD simulations. The equations are then implanted in ABAQUS in order to perform both explicit and implicit simulations. The continuum model is validated in the case of tensile test of copper single crystals for which the well known three stage curve is reproduced. Finally, FEM simulations of conical indentation are performed in copper crystals of different orientations. Comparisons with experiments give access to the initial dislocation density.
Marcel Berveiller Arts et Métiers ParisTech Metz INP	**Chapter 1: Fundamental equations of the micromechanics** This first chapter introduces the different possible microstructures of heterogeneous materials. The different origins of thermo-mechanical inhomogeneities are highlighted like the chemical, physical, and, crystallographic inhomogeneities, or, lattice defects. Then, different classes of heterogeneous materials are presented (composites, polycrystalline, multiphase materials), as well as, the topological and morphological description, the notion of representative volume element (RVE), and, the volume fractions. In this lecture, the basic equations of continuum mechanics used in micromechanics of solids are also recalled such as: stresses, equilibrium conditions, boundary conditions, volume forces. The kinematics in the small perturbation hypothesis is recalled (Displacement, distortions, rotations, compatibility conditions). Fundamental energy principles (Minimum energy principle, complementary energy principle) and Mandel-Hill condition are introduced.

Stéphane Berbenni LPMM-CNRS, ENSAM CER Metz Technopole	**Chapter 2: Heterogeneous linear elastic media with defects (eigenstrains)** In the second chapter, the relevant notion of “eigenstrain” is introduced and a complete formulation for an infinite heterogeneous linear elastic solid with eigenstrains is presented. The formulation is written under Navier type partial differential equations, and, the transformation into an integral equation using Green functions for infinite homogeneous media is described. The essential properties of Green functions and Kröner modified Green functions are detailed. This general formulation allows treating two elementary problem applications: The first one is the problem of heterogeneous and incompatible ellipsoidal inclusions (Eshelby, Kröner,) leading to the estimations of 2nd order internal stresses in a heterogeneous material; The second one is the derivation of the distortion field of dislocations like pure edge, screw dislocations or dislocation loops. Some applications useful in materials and composite sciences are also described through pile-ups of dislocation loops at grain boundaries, pairs of inelastic inclusions, interfacial operators and coated inclusions.
Véronique Favier LIM, Arts et Métiers ParisTech Paris	**Chapter 3: Homogenization methods for media with simple and complex behaviours (elastic, elastic-plastic, visco-plastic, elastic-viscoplastic heterogeneous materials)** The chapter 3 is dedicated to homogenization techniques based on the calculation of the Eshelby inclusion (seen Chapter 2). In the first section, we develop different methods of determining the effective properties of elastic heterogeneous materials. We analyse more precisely the Voigt model, the Reuss model, the Eshelby model, the Mori-Tanaka model and the classical self-consistent model. We compare the results in a two phase elastic composite with incompressible phases to assess the validity and accuracy of these methods. If one or more of the heterogeneities in a heterogeneous medium is no more linear elastic (elastoplastic,elasto-viscoplastic, etc.), the overall behaviour will be non linear. In these cases, the determination of the overall properties is more complex. The main difficulty is to well-model the elastic-

	inelastic mechanical interactions between the heterogeneities. Historically, the homogenization methods for inelastic behaviour were developed mainly for crystalline materials. The grains (single-crystal) were considered as the heterogeneities and the aim was to relate the mechanical response of a polycrystal to the fundamental mechanisms of single-crystal deformation. The second section of the chapter deals with the homogenization techniques for inelastic behaviours. First, we establish the constitutive equations for single-crystal using crystal plasticity theory and a viscoplastic framework. Second, we introduce various homogenization methods to relate the single-crystal behaviour to the polycrystal's one accounting for the mechanical interactions between grains. These homogenization methods are extended from the linear elastic case of the inelastic cases using linearization procedures (tangent, affine). Third, we finally discuss the case of linear and non linear elastoviscoplastic behaviours where complex time-space couplings involved so that long memory effect appears.
T. Böhlke, K. Jöchen, T.-A. Langhoff Chair of Continuum Mechanics University of Karlsruhe (TH) Kaiserstr. 10 D76131 Karlsruhe, Germany	**Homogenization methods for anisotropic linear elastic polycrystals** The elastic properties of uniform polycrystalline materials without defects depend on both the constitutive properties of the constituents and the microstructural characteristics like the distribution of grain orientations and grain shapes. For an overview concerning the homogenization of elastic properties see, e.g., [1]. The elementary bounds by Voigt and Reuss take into account only the volume fraction information of microstructure and hence are insensitive with respect to any morphological aspects of the grain structure. In the presentation we discuss new anisotropic Hashin-Shtrikman bounds for aggregates of cubic and hexagonal crystals. In the case of anisotropic crystallographic symmetry and isotropic morphology, an explicit form is obtained which is nonlinear in the texture coefficients. For anisotropic morphology however, the result is obtained only numerically and shows a significant influence of two-point correlation function. Furthermore, we derive a new higher-order estimate of the effective elastic properties in terms of tensorial one-point and two-point correlation functions for the special case of uncorrelated grain shapes and grain orientations [2]. Based on the integral equation formulation, a series expansion for the effective elastic properties is used as starting point [3]. We especially consider the coupling terms that arise due to the interaction of the inhomogeneous distribution of crystal orientations and non-equiaxed grain geometry. The new bounds and estimates are used for prediciting the effective and apparent properties of metals and ceramics.

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Horst Vehoff Universität des Saarlandes	**Messmethoden zur Charakterisierung innerer Grenzflächen und zur Versetzungsnukleation – vom Stahl zum nanokristallinen Werkstoff** In der Vorlesung werden hochauflösende Messmethoden zur Charakterisierung der Wechselwirkung zwischen Versetzungen und Rissen mit Korngrenzen beschrieben. Dies sind in-situ Methoden im REM (Rasterelektronenmikroskop) und RKM (Rasterkraftmikroskop). Ferner Beugungsmethoden zur Messung der Orientierung, von Versetzungen und plastischen Zonen wie EBSB (electron back scattering diffraction), ECCI (electron channeling contrast imaging) und Messungen des Orientierungsgradienten. Im letzten Teil werden noch Druckversuche an mikroskopischen Proben im nanoindentierenden REM und über Methoden der Durchführung von mechanischen Experimenten an mikroskopisch kleinen Proben in verschiedenen Umgebungen besprochen
Walter. Arnold* Department of Materials Science and Technology Saarland University, Campus D 2.2, D-66123 Saarbruecken, Germany	**Materials Characterization by Non-Destructive Testing Techniques** Components and semi-finished products are often tested for quality assurance by non-destructive testing and evaluation (NDT&E) using ultrasonics, X-ray, eddy current, thermal methods, micromagnetic techniques, and other NDT techniques. In ultrasonics, depending on the geometry and nature of the defect, volume, surface and guided waves are employed. For the reception and evaluation of the ultrasound signals reflected by the flaws, synthetic aperture techniques, ALOK, phased array are applied in addition to the standard pulse-echo technique.

*Present address: 1. Phys. Institut Universität Göttingen, Fritz-Hund Platz 1, 37077 Göttingen, Germany	This contribution discusses the physical bases of various ndt-techniques, in particular ultrasonics and micromagnetics for different applications such as testing of pipelines, railway wheels, automotive components, components made of high-strength ceramics, and electronic components. Furthermore, methods for the non-destructive characterization of materials, e.g. measurement of the hardening depth in steel and sound-velocity measurements for the determination of mechanical stress, the fatigue and creep state of materials are discussed as well. High-resolution of acoustic microscopy based on atomic force microscopy is presented allowing one to study the elastic and inelastic interaction of ultrasound with the micro- and nanostructure of a material, here nanocrystalline materials and metallic glasses. A large part of the measurements on which the presentation is based was carried out with colleagues at the Fraunhofer Institute for Non-Destructive Testing (IZFP) in Saarbrücken, Germany, and with many students from the Saarland University, Department of Materials, where the author worked until retirement.	
Stefan Diebels & Michael Johlitz Universität des Saarlandes Lehrstuhl für Technische Mechanik D- 66123 Saarbrücken e-mail: s.diebels@mx.uni-saarland.de m.johlitz@mx.uni-saarland.de	**Experimental investigation and continuum mechanical modelling of size effects in polymer layers** During the last decades glueing became a popular joining technology especially in light weight construction. In order to allow for an appropriate description of glued components in simulations the behaviour of polymer layers hast to be investigated experimentally and theoretically. In this presentation the mechanical behaviour of polyurethan layers is studied in shear experiments. As expected, it is found that the polymer behaves viscoelastic. Furthermore, if the layer thickness is varied, the experiments show a strong size effect, i. e. the effective stiffness of the specimen depends on the layer thickness. In contrast to the size effects documented in literature thin layers behave weaker than thick layers. From the physical point of view the formation of interphases between the polymer and the substrate is responsible for this behaviour. In a first part of the presentation the experimental setup of classical tension tests and of the above mentioned shear tests is discussed. The experimental results are presented for different loading rates	

	showing viscoelastic effects. In order to minimize the experiments isothermal conditions are applied. Based on the results of the tension tests the concepts of viscoelasticity are motivated starting from a simple rheological model. The model consists of a spring (Hooke element) and a spring-dashpot combination (Maxwell element). This model is able to describe the essential properties of viscoelastic materials, i. e. kreep and relaxation can be captured in an appropriate way. In a second step the model is extended towards a threedimensional continuum mechanical model taking into account finite viscoelasticity. It is shown how the ideas of the rheological model are transfered to the finite model. For the presented model the thermodynamical consistency is shown. A model formulated in the framework of classical continuum mechanics is not able to predict size effects. Therefore, an extension of the classical approach is motivated. An additional structural parameter is introduced which describes the local variation of the material properties in the polymer layer. Combining this extension with the concepts of finite viscoelasticity yields an extended model which is able to describe the experimentally observed effects. An appropriate strategy for the parameter identification is proposed and it is shown that the involved model parameters can be quantified based on the experimental results.
Samuel Forest Mines ParisTech Centre des Matériaux CNRS UMR 7633 BP 87 91003 EVRY e-mail: samuel.forest@ensmp.fr	**Mechanics of Generalized Continua with Application to Multiscale Phenomena** The classical Cauchy continuum mechanics can be extended to incorporate additional microstructural features of materials and account for some observed size effects in the materials' behaviour. Two main enhancements are possible and will be presented in two lectures: • Gradient Theories. The size-independent continuum mechanics of materials is based on the strain tensor, i.e. the symmetric part of the gradient of the displacement field. Introducing the second and third gradients of the displacement field makes it possible to describe size-dependent stress concentration, and surface tension effects. The corresponding theories elaborated by Mindlin [1] will be presented and applied to molecular dynamics effects in crystalline solids. Some size effects observed in the plastic behaviour of metals can be

modelled by introducing the dislocation density tensor which is directly related to the gradient of plastic strain. This extension of crystal plasticity will be presented based of the framework established by Gurtin [2].

- Micromorphic Media. The classical continuum can also be extended by introducing additional degrees of freedom representing the deformation of microstructural elements. The micromorphic model by Eringen and Mindlin represents a versatile theory that can be applied to the size-dependent mechanics of composites and of plastic crystalline solids. In composites, the micromorphic theory is applicable at the limit of the hypothesis of separation of scale. In crystalline solids, the micromorphic model is closely related to the previous strain gradient plasticity models [3].

References

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