CMM-SolMech 2022 conference

S08 Nanomaterials and nanocomposites, their properties and applications

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A NEW CONCEPT OF EPOXY RESIN COMPOSITE DOPED WITH CARBON-BASED NANOPARTICLES: MANUFACTURING, EXPERIMENT AND MODELING

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Our studies investigated the elastic-plastic properties and strength of epoxy resin matrices promoted with different concentrations of carbon-based nanomaterials.
Multiwall carbon nanotubes (MWCNT) and graphene nanopowder xGNP-M-5 (XG Science), in the manufacture of epoxy L20/graphene composites, specific amounts of resin were mixed with hardener and graphene and oxidized graphene in 0.1, 0.5, 1, 2.4% by weight, prepared. The resulting mixtures were degassed under vacuum (-1 bar) and poured into silicone molds. The composites were left in the fume hood to cure for 24 hours and then heated at 120°C for 96 hours. A similar procedure was used for the fabrication of MWCNT/Resin composite.
The mechanical response of epoxy networks was investigated under uniaxial tension and compression at low strain rates, using the MTS 858 testing machine and the DIC (Digital Image Correlation) technique. In the quasi-static uniaxial compression tests, cylindrical specimens with the dimension ratio of 1.5: 1 (height: diameter) were used. In the axial tensile tests, flat samples cut from lamellas with a thickness of 1 mm were used. The actual stresses and actual strains were determined, assuming the incompressibility of the material. The tests were carried out on at least three samples for each type of epoxy graphene composites. Young's modulus was determined for the linear part of the stress-strain relationship for strains ranging from 0.1 to 0.3%. The resin's deterioration process results from developing a multiscale micro-shear bands system leading to inelastic strains terminated by cracking in samples with deformation of 4% resulting in a sharp drop in stress. Based on these observations, a model describing the inelastic behavior of nanocomposite was proposed, modifying the viscoplastic flow equation by introducing the shear banding contribution function.

CRITICAL THICKNESS EVOLUTUTION DURING THE SUBSEQUENT EPITAXIAL LAYERS GROWTH

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The effect of bending of threading dislocations as well as the effect of the nucleation of dislocation half-loops at the surface of growing layer are discussed. A brief overview of several papers [1,2,3,4] which in the speaker opinion had a significant impact on the mathematical prediction of critical thickness of thin layers is presented.

The analysis concerns the critical thickness of (i) the first layer deposited directly on bulk crystal as well as the critical thicknesses of (ii) a layer grown on the previously deposited layers. The critical thicknesses of subsequently deposited layers can differ significantly from each other. Moreover, the capping of open layer changes its critical thickness too. In result, the misfit dislocations already formed at the bottom of uncapped layer can stand again up to the threading position during the capping. The consequences of such a mode of crystal growth on the resultant quality of thin layers are discussed.

Another question discussed is the prediction of various critical thicknesses below which the given layer must be grown to save its good quality. In some specific cases, the layer quality can be damaged by: (i) phase transition, (ii) fracture and/or (iii) misfit dislocations formation. Each of phenomena mentioned results its own critical layer thickness, and in order to obtain a good quality superlattice none of critical thicknesses should be overcome during the growth.

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DESIGN OF NANOSTRUCTURES BASED ON MOLYBDENUM

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2D materials play important role in modern material science. Apart from graphene [2] based on carbon there is possible to create new 2D materials based on molybdenum. One of the most prominent 2D material is the Molybdenum Disulfide (MoS2), which reveals polymorphism at the nanolevel. The 2H phase has semiconducting properties and approx. Young's modulus equals to 130 N/m, while the 1T polymorph reveals metallic or ferroelectric properties and two times lower stiffness [3]. Both phases of MoS2 can exist simultaneously [4]. This paper presents an optimization approach enabling to obtain MoS2 heterostructures with desired mechanical properties. The proposed memetic approach combines the global optimization, based on the bio-inspired algorithms (e.g. evolutionary algorithm) with the local conjugated-gradient minimization of the potential energy of the nanostructure [2]. The behavior and energy of the atoms is determined by the REAX-FF potential [1,3].
Memetic optimization of MoS2 with presence of defects in the form of missing S atoms or the substitution of Mo atoms in place of S is also considered. The MoS2 structure is modelled with the use of LAMMPS software and the Stillinger-Weber interatomic potential is used

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DEVELOPMENT OF CONSTITUTIVE RELATIONS OF VISCOPLASTICITY ACCOUNTING FOR SHEAR BANDING

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Two types of shear banding mechanisms control viscoplastic flow in solids.
The instantaneous multiscale shear banding system formed by micro-shear bands of the thickness of the order of 0.1 micrometer, the clusters of micro-shear bands producing the discontinuity of the microscopic velocity field vm and the macroscopic zone of shear strain localisation spreading through the representative volume element (RVE) of a polycrystalline metallic solid. A new concept of the RVE with strong singularity was introduced, and the instantaneous shear banding contribution function was defined [1].
The cumulative organisation of micro-shear bands is based on the accumulation of the particular contribution of micro-shear bands forming clusters in specific volumes contained in RVE. The micro-shear bands gradually contribute to the development and growth of micro-shear bands clusters. Finally, the clusters accumulate in the macroscopic localisation zone spreading across the macroscopic volume of considered material. Such deformation mechanism is observed in amorphous solids such as glassy metals or polymers, particularly epoxy resins. Micro-shear bands are growing from the local shear transformation zones (STZ). Finally, the phenomenological viscoplasticity model introduces the cumulative shear banding contribution function [1].

Both types of the mentioned shear banding mechanism appear with a variable contribution in the course of deformation processes. This situation may occur in polycrystalline metallic solids, subjected to the deformation characterising by a distinct change of deformation or loading paths. Also, materials that reveal the hybrid structure of amorphous, ultra-fine grained and nanostructural phases are prone to the mixed shear banding responsible for inelastic deformation. Finally, the description of the inelastic behaviour of epoxy resin composite doped with carbon-based nanoparticles was specified, modifying the viscoplastic flow law by determining the shear banding contribution function [2].

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SPECIFIC PROPERTIES OF NANOMATERIALS AND THEIR POTENTIAL IN TECHNICAL APPLICATIONS

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Nanomaterials can generally be divided into single nanoparticles and two- and three-dimensional structures based on them. In my talk, I will address nanomaterials' structural, electronic, and mechanical properties that make them superior to traditional materials. The current state of research and the range of applications of nano-materials, their possible applications based on nanoparticle selection, manufacturing processes, particle size and composition, and the influence on their mechanical properties are presented and discussed using examples. This underlines the growing future importance of nanomaterials in the development and application of materials science.