DFG-Project Schm 746/88-1

Numerical optimization of bio-inspired ceramic material systems

Begin of the project: 01.12.2009

End of the project: 31.08.2013

Summary:

To get a better insight and understanding concerning the mechanical behavior of bio-inspired layered materials consisting of oxide ceramics (Titanium dioxide, TiO_2) and organic layers (Polyelectrolyte, PE), numerical and analytical methods and models are applied on the microscopic scale. The investigations are concentrated on the elastic properties of the ceramic phase, the viscous behavior of the organic phase as well as the interlayer properties and the single layer dimensions and their influence on the elasticity, hardness and ductility of the bio-inspired layered structures. Finite Elements simulations of nanoindentation and tensile tests have been performed of the layered nanocomposite (see Fig. 1 right) in order to derive the mechanical properties of the nanocomposite and of the pure components. In Figure 2 one example of a nanoindentation simulation of a nanocomposite with a 10 nm thick layer of PE is presented. The influence of the thickness ratio of the organic phases on the hardness and Young's modulus on the layered nanocomposite are analyzed.

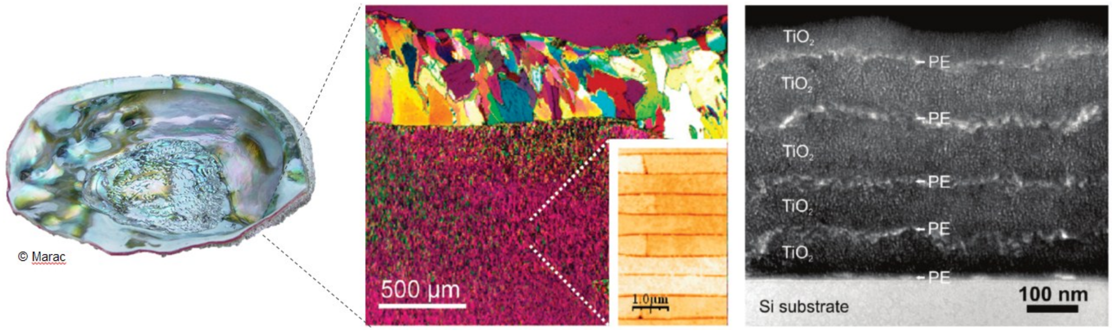

Fig. 1: The shell of an Abalone and the detailed view of it. Nacre, a part of the shell composed out of protein and Aragonite, which is interesting for its mechanical properties, is shown in even more detail in the yellow colored magnification. On the right a microscopy picture of artificial nacre is shown. The different layers and the substrate are marked.[1]

[1]Burghard, Z.; Zini, L.; Srot, V.; Bellina, P.; van Aken, P.A.; Bill J., Toughening through nature-adapted nanoscale design, Nano letters 2009 American Chemical Society, 9(12), 4103 8.

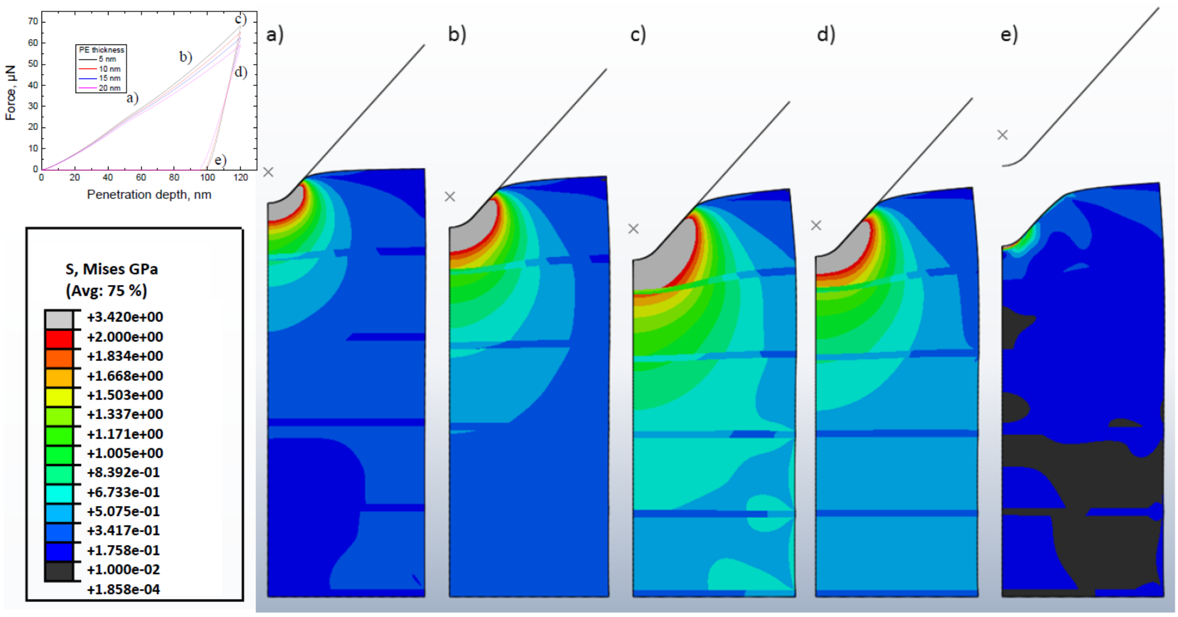

Fig. 2: Contour plots of von Mises stresses at different stages of simulation of a nanoindentation test of a five-fold layered TiO_2/PE-nanocomposite, the layer thickness of TiO_2 is 100 nm and the layer thickness of PE is 5 nm. a) and b) show two stages of the beginning of the indention process, c) shows the maximum depth of the indenter and d) and e) show two stages of relaxation during unloading of the material. The stress is distributed up to the base of the model. The figure in the left upper corner shows the stages a) to e) on the Force-Penetration curve (with different PE-layer thicknesses).

The modeling of the material behavior of composites is generally based on a model for the behavior of each constituent or phase of the composite. For the calculation of the nanoindentation behavior of a layered TiO_2/PE structure the stress-strain curves of both phases (TiO_2 and PE layer) are required. For the definition of the stress-strain behavior of the constituents a own developed methodology involving the combination of nanoindentation technique and Finite Element Method to characterize the mechanical (elastic and plastic) behavior of the titanium oxide thin film is applied. An example for a parameter study is shown in Fig 3a compared to the experimental results.

Based on the results of the parameter study, the simulations of the nanocomposite can be conducted. Compared with the experimental results, it shows a difference in the Young's modulus. With incorporation of the concept of mineral bridges, (which are structures in natural nacre that connect two layers of Aragonite) the resulting Force/Penetration curves of the nanoindentation experiment can be explained and simulated. The results of the simulations and the results of the analytical model with mineral bridges are presented in Fig. 3b.

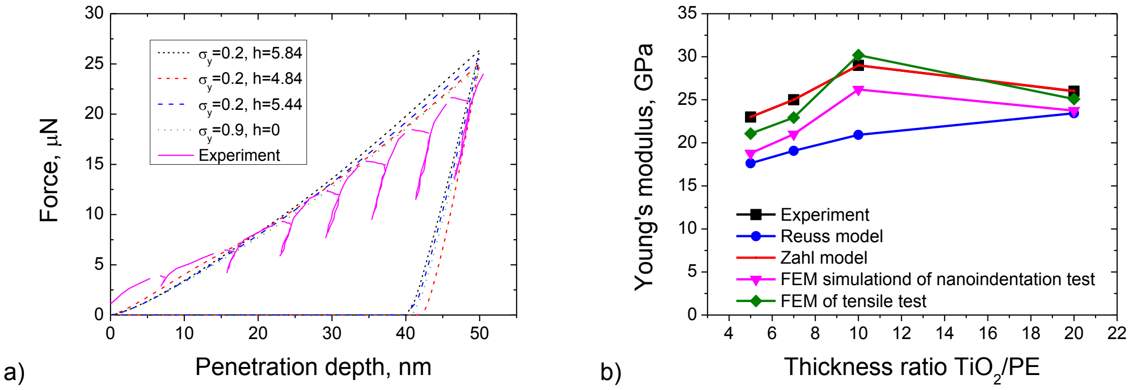

Fig. 3: Parameter studies of mechanical properties of the constituents of the artificial nacre using continuum mechanics methods: a) The comparison of Force-Penetration curves, obtained from nanoindentation experiments (continuous line) and from FE-simulations with a variation of parameters: Young's modulus E = 27 GPa and yield stress σ_y = 0.2 GPa and variation of work-hardening coefficient: h = 5.84, 4.84 and 5.44 GPa; b) The dependence of the Young's modulus of the layered TiO_2/PE-nanocomposite on the thickness ratio of the constituents. The comparison of the experimentally defined Young's modulus with the one derived from FE-simulations of nanoindentation test. All models include mineral bridges with a very high Young's modulus of 282 GPa (experimental curve and the curve calculated with the Zahl et al. model are overlapping).

As can be seen, at all volume fraction ratios of the layers, the results show good qualitative agreement with the experimentally gained results but the nanoindentation simulation underestimate the Young's modulus as obtained in the experiments and from the analytical model with taking into account the same volume fraction of mineral bridges. This can be attributed to the complex state of stress during indentation and the anisotropic nature of the layered material. For the verification of the results obtained from FE-simulations of the nanoindentation tests, the tensile test experiments have been simulated with the same volume fraction of mineral bridges.

Future works will concentrate on the influence of the thickness ratio of the layers on crack propagation and crack prevention.

Project Partner:

- Department of Zoology, Institute for Biology
- Department of Molecular Biology and Plant Virology, Institute for Biology
- Institute for Technical Biochemistry
- Institute for Material science

For further information see also: http://www.bionik.uni-stuttgart.de/

Publications:

1. Galina Lasko, Zaklina Burghard, Immanuel Schäfer, Siegfried Schmauder, Ulrich Weber and Dieter Galler, Definition of stress-strain behavior of bio-inspired layered TiO2/PE-nanocomposite by inverse modeling based on FE-simulations of nanoindentation test, Molecular & Cellular Biomechanics special issue (2012), accepted (in Press).

2. Galina Lasko, Zaklina Burghard, Joachim Bill, Immanuel Schäfer, Siegfried Schmauder, Ulrich Weber, Simulation of mechanical properties of bio-inspired TiO2/PE nanocomposites, Advanced Engineering Materials, (2012), accepted. (in Press).

3. Immanuel Schäfer, Galina Lasko, Tuan Anh Do, Jürgen Pleiß, Ulrich Weber, Siegfried Schmauder, Peptide - Zinc oxide interaction: Finite Element Simulation with cohesive elements based on molecular dynamics simulation, (2013), Work in Progress.

Conference presentation:

1. Simulations of mechanical properties of bio-inspired TiO2/PE-nanocomposites, International Conference on Computational & Experimental Engineering and Sciences (ICCES) 2012, 30 April- 4 May 2012, Crete, Greece

Conference poster presentations:

1. Numerical optimization of bioinspired ceramics material systems at the international one-day Workshop "Prospects of Bionics for functional Materials Science and Engineering", 22 September, 2010, Leoben, Austria

2. Numerical optimization of bioinspired ceramics material systems at the international symposium "Molecular Bionics-From biomineralization to functional materials" 3-6 October 2010, Schloss Ringberg, Rottach-Egern, Germany

3. FEM-Simulation der mechanischen Eigenschaften bionisch inspirierter TiO_2/PE Nano-Verbundwerkstoffe at the Jahrestagung der Deutschen Gesellschaft für Biomaterialien 2011, 10-12 November 2011, Gießen, Germany

4. Simulation der mechanischen Eigenschaften von bio-inspirierten TiO_2/PE Nanoverbundmaterial at the 6. Bionikkongress „Patente der Natur" 26-27 October 2012, Bremen, Germany

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