21st Nordic Seminar on Computational Mechanics
NSCM-21
T. Kvamsdal, K. M. Mathisen and B. Pettersen (Eds.)

THREE-DIMENSIONAL FINITE ELEMENT STUDY ON THE NANOINDENTATION PROCESS OF HYDRATED NACRE

J. ZHAO[*†], Z.L. ZHANG[*]

[*] Department of Structural Engineering (DSE)
Norwegian University of Science and Technology
N-7491 Trondheim, Norway
e-mail: junhua.zhao@ntnu.no, zhiliang.zhang@ntnu.no

[†] Institute of Nano Science (INS)
Nanjing University of Aeronautics and Astronautics
210016 Nanjing, China
Email: jhzhao@nuaa.edu.cn

Key words: Nacre, Nanoindentation, Hardness, Finite Element Simulation.

Summary. The nanoindentation process of hydrated nacre has been simulated using three-dimensional finite element method. The constitutive relation is based on Barthelat et al's (Journal of the Mechanics and Physics of Solids, 2007, 55: 306-337) test results. The influence of the maximal loading on the simulation process is taken into account. The nanoindentation process and hardness of nacre are compared with other experimental results. It is shown that the hardness from finite element simulation is always higher than that of experiment and it gradually approaches to the experimental one with the increase of the maximal loading.

1 INTRODUCTION

In the past years, the mechanical properties of nacre have become very attractive to material engineers as well as chemical and physical scientists because of the fantastic strength and ductility of natural nacre. The natural nacre is composed of about 95% inorganic aragonite phase and only a few percent of organic biopolymer mortar in form of hierarchical structural architecture extending over several distinct length scales[1-10].

In this paper, the nanoindentation process of hydrated nacre has been simulated using three-dimensional finite element method. The constitutive relation is taken from Barthelat et al's[10] test results.

2 FINITE ELEMENT MODELING

The nanoindentation process is a three-dimensional elastic-plastic large strain static problem. It must be simultaneously considered for the nonlinear material behaviour, geometry and contact condition. Here the standard Berkovich indenter with tip curvature radius 80nm [9] is used. The real tip curvature radius of an indenter varies from 50 to 100nm between a new and used one. Due to the symmetry of the problem, only 1/6 of the model is considered in the analysis. The solutions are performed by the use of the commercial code ANSYS (version 8.0) with 20-noded isoparametric elements. A typical FE meshes and the geometrical relationship between Berkovich indenter and the indented section are illustrated in Fig. 1. The mesh refinement is enforced close to the contact region, and about 10000 elements are used in the analysis.

(a) (b)

Fig.1 (a) Typical finite element meshes of the 1/6 indenter and nacre. (b) The geometrical relationship between Berkovich indenter and the indented section.

In the calculations, Young's modulus of the indenter is taken as an order of magnitude higher than that of indented material, and Poisson's ratio 0.1 is used[9]. The hydrated nacre is assumed to be an isotropic power hardening material and the material constants are fitted using Eq. (1) from Barthelat et al's[10] test results. The fitting results are shown in Fig. 2, and Poisson's ratio of the hydrated nacre is taken as 0.3.

For the hydrated nacre, the constitutive relation is fitted as

$$\begin{cases} \varepsilon = \dfrac{\sigma}{E}, \ (\sigma \le \sigma_{ys}) \\ \varepsilon = \dfrac{\sigma}{E}\left(\dfrac{\sigma}{\sigma_{ys}}\right)^{n-1} \end{cases} \tag{1}$$

where Young's modulus E=85GPa, the yielding stress σ_{ys}=60MPa, the strain hardening exponent n=6.68.

For the dry nacre and pure aragonite, both are close to the linear materials. The Young's moduli of the two materials are fitted as 91.22GPa and 111.88GPa, respectively. Obviously, the stiffness of dry nacre and pure aragonite is a some what higher than that of hydrated nacre, while their toughness is much lower[11].

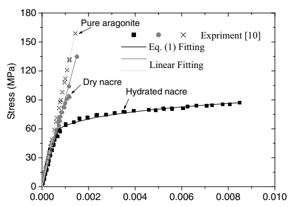

Fig.2 Stress-strain curves of nacre and pure aragonite in tension along the tablets.

No friction is considered in the simulation process, because the friction coefficient has minor influence on the results[9]. The thickness and radius of the indented section is chosen

1 m and 4 m respectively in order to ensure that the stress-free boundary conditions have negligible effects on the stress state.

3 RESULTS AND DISCUSSIONS

The finite element results are compared with that of the experiment in Fig. 3. The loading increment of every step is adjusted by finite element programme itself, which can greatly improve efficiency of calculation and have no effect on the results. It is interesting to find that the agreement is fairly good, except a small difference which may arises from several sources. First, the constitutive relation is taken from ref. [10], but the nanoindentation process is used in ref. [11] here. Second, the isotropic nacre is considered in the calculations, the real nacre is an anisotropic material.

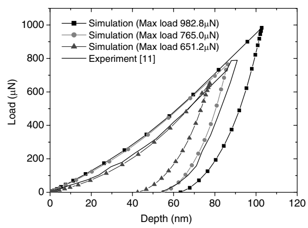

Fig. 3 Comparison of test and finite element simulation

The hardness can be obtained using the method in ref. [9, 12]

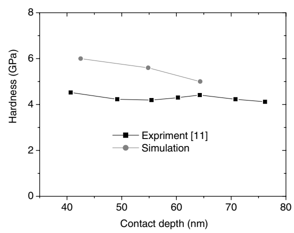

Fig. 5 Comparison of the hardness of test and that of finite element simulation

As shown in Fig. 5, the hardness from finite element simulation is always higher than that of test. When the maximal load increases, the numerical hardness approaches to that of test.

5 CONCLUSIONS

- The three-dimensional elastic-plastic finite element can be used to simulate the nanoindentation process of nacre well. The numerical harness is found to be always higher than that of test. When the maximal load increases, the numerical hardness becomes closer to that of test.

REFERENCES

[1] A.G. Evans, Z. Suo, R.Z. Wang, et al, “Model for the robust mechanical behavior of nacre”, J. Mater. Res., **16**, 2475-2484 (2001).

[2] R.Z. Wang, Z. Suo, A.G. Evans, et al, “Model for the robust mechanical behavior of nacre”, J. Mater. Res., **16**, 2485-2493 (2001).

[3] H. Gao, B.H. Ji, I.L. Jager, et al., “Materials become insensitive to flaws at nanoscale: Lessons from nature”, PNAS, **100**, 5597-5600 (2003).

[4] A. Lin and M.A. Meyers, “Growth and structure in abalone shell”, Mater. Sci. Eng. A, **390**, 27-41 (2005).

[5] M. Rousseau, E. Lopez, A. Coute, et al., “Sheet nacre growth mechanism: a Voronoi model”, J. Struct. Bio., **149**, 149-157 (2005).

[6] D. Katti, K. Katti, “Modeling microarchitecture and mechanical behavior of nacre using 3D finite element technique”. J. Mater. Sci., **36**,1411-1417 (2001).

[7] F. Barthelat, H.D. Espinosa, “Elastic properties of nacre aragonite tablets”, Proceeding of the 2003 SEM Annual Conference and Exposition on Experimental and Applied Mechanics, June 2-4, Charlotte, North Carolina, Session 68, Paper 187, 2003.

[8] C. Liu, W. Li, H. Li, “Simulation of nacre with TiC/metal multilayers and a study of their toughness”, Mater. Sci. Eng. C, **4**, 139-142 (1996).

[9] M. Li, N. Liang, T. Zhang, L. Wang, “3D finite element simulation of the nanoindentation process”, Acta Mecha. Sin., **35**, 257-264 (2003).

[10] F. Barthelat, H. Tang, P. Zavattieri, et al., “On the mechanics of mother-of-pearl: A key feature in the material hierarchical structure”, J. Mech. Phys. Solids, **55**, 306-337 (2007).

[11] X. Li X , W. Chang, Y. Chao, et al., “Nanoscale structural and mechanical characterization of a natural nanocomposite material: The shell of red abalone”, Nano Lett., **4**, 613-617 (2004).

[12] W. Oliver, G. Pharr, “An improved technique for determining hardness and elastic modulus using load and displacement sensing indentation experiments”, J. Mater. Res., **7**, 1564-1583 (1992).