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Inhomogeneous Domains, Dynamic Loads: Toward Simulation of Mechanical Damage in Realistic Microstructures

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OVERVIEW OF EFFORTS Simulations were performed to assess the effect of juncture properties on mechanical response of point-bonded fibrous networks. The transport properties were simultaneously assessed. A series of numerical implementations were devised through support by this program, and advancement in simulations of materials particularly relevant to battery technology was made. Two publications are in progress whose efforts were supported by this project, and several presentations were also made with support from this program.

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PUBLICATIONS WITH WORK SUPPORTED IN PART OR WHOLE BY ARO

in preparation, Wang, C.W., Berhan, L. and Sastry, A.M., "Mechanics of Stochastic Fibrous Networks," for ASME Journal of Engineerng Materials and Technology, (2000).

accepted, Cheng, X., Sastry, A.M., and Layton, B.E., "Transport in Stochastic Fibrous Networks," to ASME Journal of Engineering Materials and Technology, (2000).

PRESENTATIONS WITH WORK SUPPORTED IN PART OR WHOLE BY ARO

Department Seminar, Department of Materials Science, University of Virginia, Fall, 1999.

Invited presentation to the Ultralight Metals Study Program of the ONR MURI (M.F. Ashby, A.G. Evans, J.W. Hutchinson, N.A. Fleck, H.N.G. Wadley, co-PI's), Williamsburg, Virginia, August, 1999.

Department Seminar, Department of Materials Science, Brown University, April, 1999.

Department Seminar, Division of Engineering and Applied Science, Harvard University, April, 1999.

Department Seminar, Department of Mechanical Engineering, University of Illinois at Chicago, Chicago, Illinois, March, 1999.

Department Seminar, Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, February, 1999.

Department Seminar, Materials Science and Mineral Engineering Department, University of California, Berkeley, Berkeley, California, December, 1998.

Mechanics and Computation Division Seminar, Department of Mechanical Engineering, Stanford University, Stanford, California, October, 1998.

Department Seminar, Department of Mechanical Engineering, University of Minnesota, Minneapolis, Minnesota, October, 1998.

Main Findings

Determination of the mechanical response and damage tolerance of stochastic fibrous networks is of important for a wide range of physical applications, including the design of paper, electrochemical substrates, and web reinforcement in polymeric composite materials. In all such cases, fibers of variable length and aspect ratio are placed randomly in a plane, and fused. We may thus define the microstructure as a two-dimensional network, with key geometric features defined by statistical distributions, rather than single-valued descriptors. The connectivity of the network results from the selection of network parameters, and thus must be calculated after a network is generated via simulation, to achieve a physically realistic representation. An example is shown in Fig. 1.

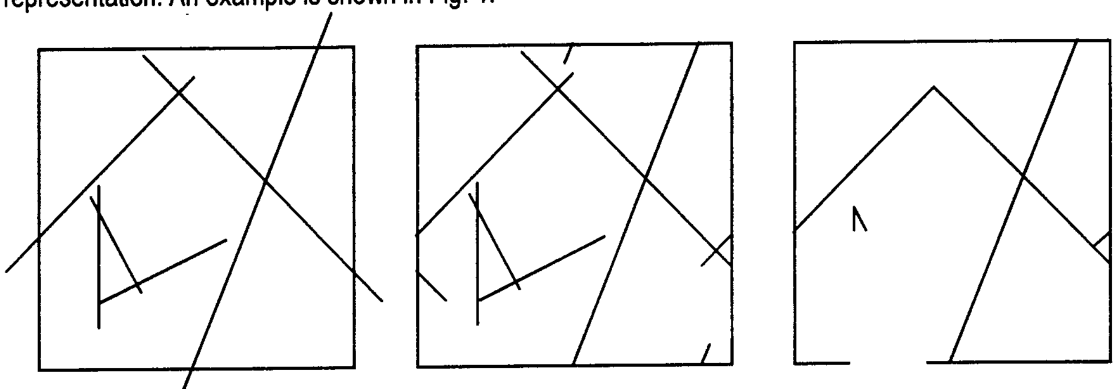

Figure 1. Network generation technique. Fibers are generated according to a known statistical distributions of length, orientation and location. Periodic boundary conditions are then enforced, and non-load-bearing structures are removed, leaving the "reduced" network for analysis.

Several key issues were examined, including the effect of order of beam theory used (Fig. 2), bond density for similar volume-fraction networks (Fig. 3), and effect of preliminary investigation of 3D effects.

Results indicated that lower order theory was appropriate for materials technologically relevant to batteries. However, preliminary results indicated a marked difference between peak loads in 2D versus 3D models. This will be a key feature of future work.

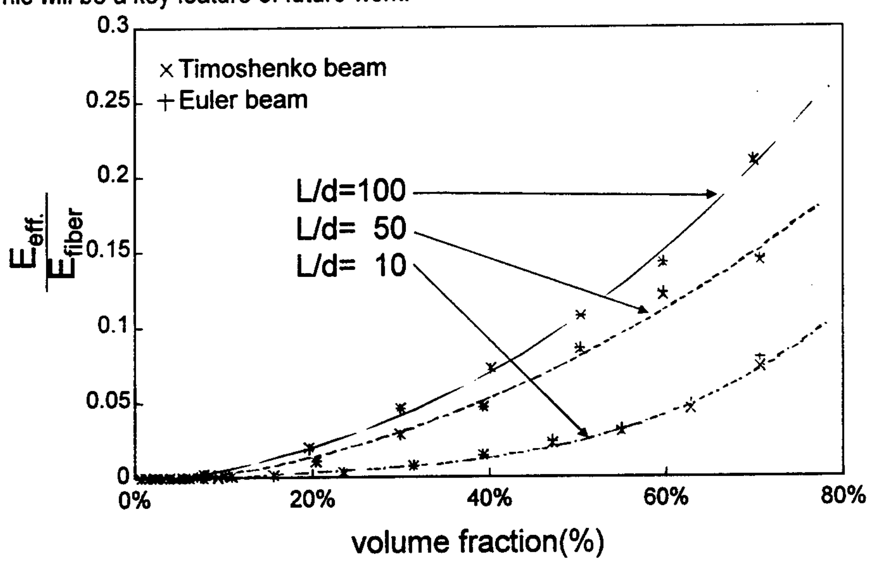

Figure 2. Comparison of the Euler beams and Timoshenko beams in simulations of effective network modulus, for a range of volume fractions and three aspect ratios (100, 50, 10).

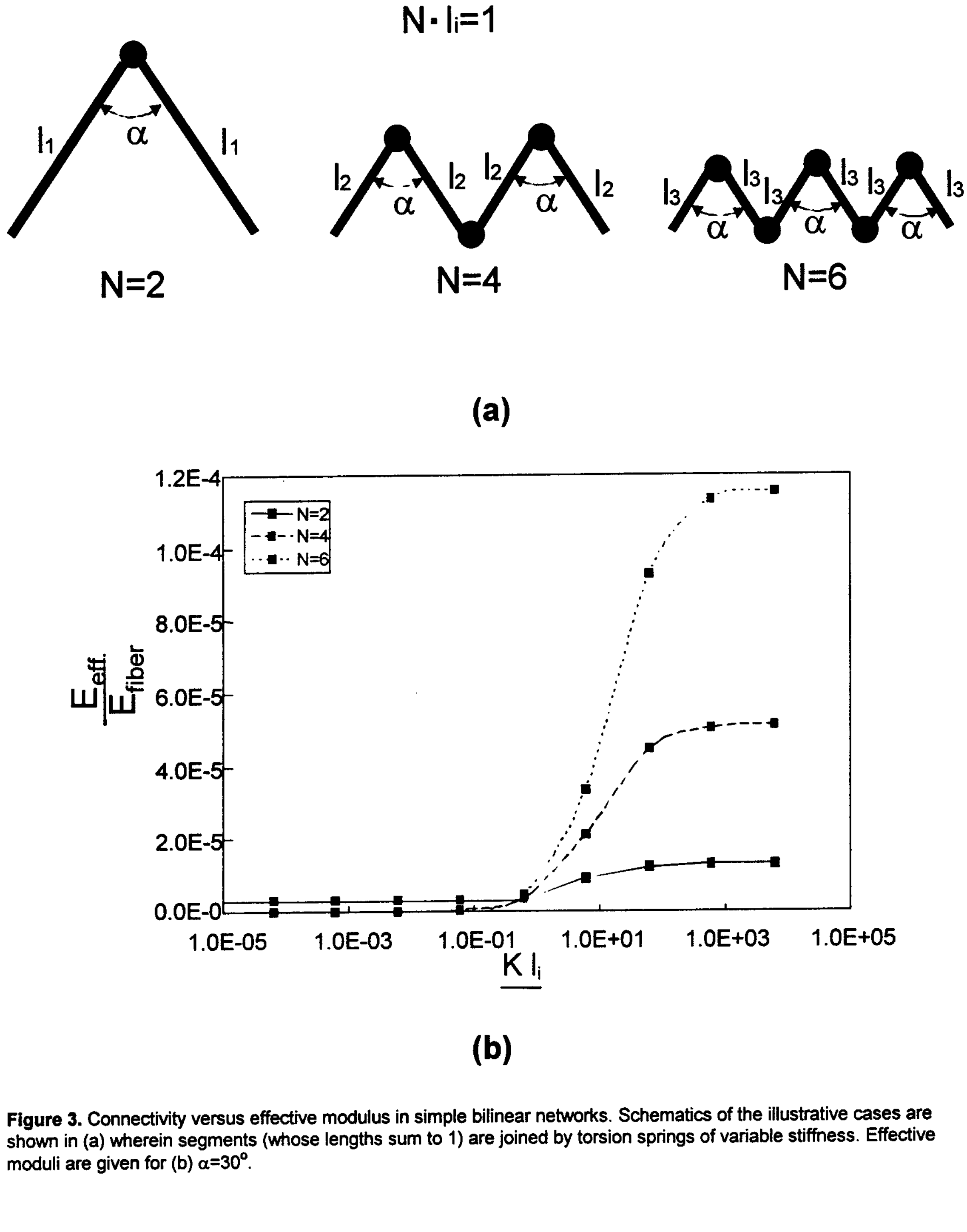

Figure 3. Connectivity versus effective modulus in simple bilinear networks. Schematics of the illustrative cases are shown in (a) wherein segments (whose lengths sum to 1) are joined by torsion springs of variable stiffness. Effective moduli are given for (b) α=30°.

IMPACT AND FUTURE WORK There is great opportunity for advancement of current technologies for failure prediction in dynamic loads in the important area of locally heterogeneous microstructure. Research is needed to quantify the shortcomings of application of both quasi-static and regular structure assumptions to these problems.

Determination was made of the scale at which image analysis and failure analysis can be effectively used to predict behavior up to failure in large volumes of materials. The materials encompassed promising structures in Ni/MH and Li-ion cells.

In the longer term (~2-5 years) it is anticipated that the addition of the large deformation mechanics to the current models will allow guidelines for development of FE structural analysis of microstructurally-designed materials. This type of analysis and simulation is necessary in order to make the technological leap from materials selection for an application, to materials design for an application. Work initiated as a follow-on to this program (supported in part by the Department of Energy) has included 3D simulations of fiber-particle and fiber-fiber bonds. This work is being rapidly expanded to allow more general guidelines for microstructural design of battery materials, and other low-density structures.