

NANOSTRUCTURED NETWORKS: MATERIALS, MECHANICS AND APPLICATIONS

Zhiping Xu

Computational Energetics Laboratory, Department of Engineering Mechanics and Center for Nano and Micro Mechanics, Tsinghua University, Beijing 100084, China

Summary Networked materials, from buckypapers (carbon nanotube networks) to cytoskeletons, feature structural hierarchies from nano to macro. With the combination of cutting-edge nano-engineering techniques and novel inspiration from biology, synthetic networked materials hold great potential in a number of applications, e.g. active, responsive, dynamic materials. In addition to the detailed properties of building blocks, interfaces and network topology, emergent phenomena also present. In this talk, we first present an analysis on the basic structural and mechanical properties of simple networks, followed by discussion on the structures, properties and transport behaviour of several networked materials, including networks of carbon nanotubes, graphene, collagen and cytoskeletons.

Keywords: nanostructures, networks, buckypaper, cytoskeleton

INTRODUCTION

Nanostructured networks have attracted much interest in various fields including physics, chemistry and biological science. [1] Sharing similar topology, examples such as cytoskeleton and buckypapers differ in the building blocks and interfacial properties. The structural information and its relation to materials properties are the keys not only to understand biological materials, but also in developing advanced materials. In this paper, we will present a comparable study on networked materials of carbon nanotubes and collagen. The structural assembly, evolution of their microstructure and mechanical properties are discussed by considering their geometry parameters, external loads, crosslinks, entanglement etc. [2-4]

MODEL ANALYSIS OF SIMPLE NETWORKS

For a network consisting of fibres, its structure and mechanical properties is defined by the building blocks, their interfaces and hierarchy of topology. Cytoskeleton and collagen fibres feature aspect ratios $a = l/D$ over hundreds, where l is the fibre length and D is the diameter. Carbon nanotubes with extremely high a values ($\sim 10^7$) are recently synthesized. For building blocks with such a wide span of geometrical characteristics, distinct mechanisms in network assembly and deformation are expected, as illustrated in Figure 1.

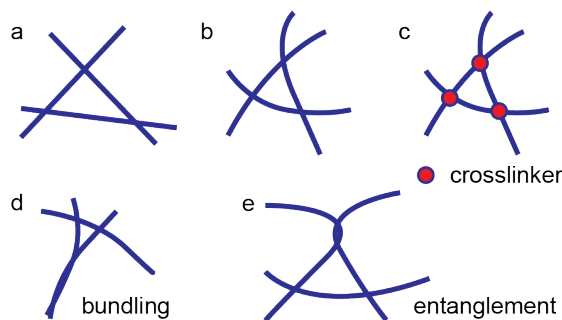


Figure 1 | Mechanisms in network assembly and deformation.

When l is shorter than the persistence length of a fiber, l_p , fibres are straight at the characteristic length scale of a network as shown (Figure 1(a)), which will change into curved shapes as l increases (Figure 1(b)). As the interfaces between fibres are crosslinked by agencies such as molecular motor in cytoskeleton networks, the networked structure can be much constrained as shown in Figure 1(c). On the other hand, some interfaces, such as those between carbon nanotubes or graphene nanostructures, are adhesive through non-covalent interactions, and fibres will aggregate into bundles as driven by the surface tension (Figure 1(d)). As l increases further beyond l_p , entanglement between long fibres will play an important role in the mechanics of networks (Figure 1(e)).

MATERIALS AND METHODS

In addition to the previous descriptive discussion on the properties of networked nanostructures and some analysis of scaling laws, we first perform atomistic simulations in supplement to clarify the structure-properties relation. Multiscale techniques including first-principles calculations, full-atom and coarse-grained molecular dynamics are used.

RESULTS AND DISCUSSION

Network structure. We find that the potential surface of nanostructured networks is complicate and corrugated. The microstructure can be stabilized at local minima at the equilibrium condition. However, as non-equilibrium driven force such as mechanical loads are introduced, significant changes in the network topology are observed. For example as shown in Figure 2, cycling loads with increasing amplitudes, the pore size of carbon nanotube networks magnified by bundling between nanotubes. These microstructures, once formed, can hardly be changed without further cues externally applied.

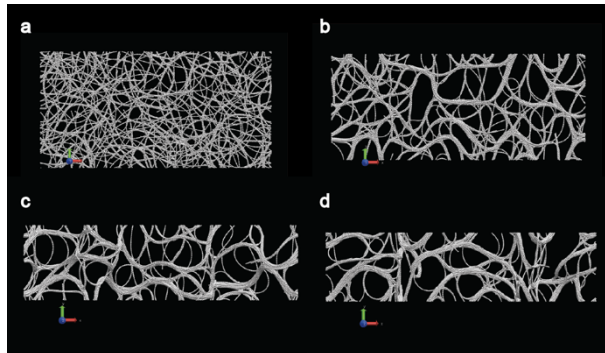


Figure 2 | Microstructure evolution under cycling loading with a maximum strain amplitude of 0.01 (a), 0.4 (b), 0.8 (c) and 1.2 (d).

Mechanical properties. The changes in network topology corresponds to different mechanical response and energy storage mechanisms. Figure 3 shows the force-strain relation (force is used instead of stress due to the significant changes in the network thickness during deformation) and mechanical energy absorption. The results show that there exists remarkable energy dissipation during the very first cycles where microstructure evolves and is stabilized. The microstructures formed at high loads feature significantly enhanced mechanical energy storage.

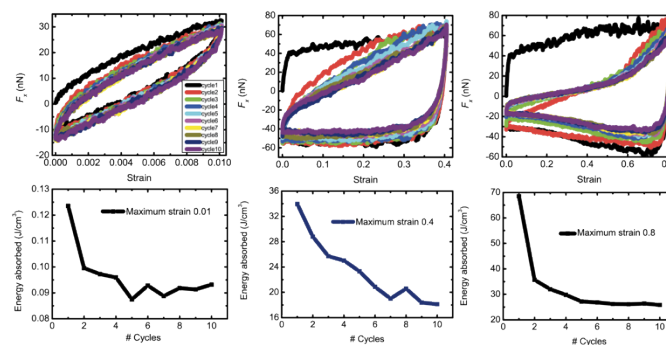


Figure 3 | Mechanical properties carbon nanotube networks. Top: force-strain relations for cycling strain loads of 0.01, 0.4 and 0.8 from the left to right. Bottom: mechanical energy absorbed as a function of loading cycles.

We will also present detailed discussion on graphene, collagen cytoskeleton networks, from a comparative point of view. Moreover, effects of crosslinks and entanglement are investigated, which show a direct link to the affinity of nanostructured networks and their mechanical properties. Transport processes related to these networks will be covered later. Several key applications in filtration and electrochemical energy storage will also be mentioned. Detailed information can also be found in Ref. [2-4].

CONCLUSION

In this paper, we discussed the structures and properties of nanostructured networks, using several materials including buckypapers as examples, with special focuses on not only the properties of the building blocks and their interfaces, but also their responses to external cues such (mechanical loads etc.) and nano-engineering techniques such as crosslinking. The results and conclusion presented here could pave the way for the rational design and optimal development of future active, responsible and dynamic materials.

REFERENCES

- [1] P. de Gennes, *Scaling Concepts in Polymer Physics*, Cornell University Press, 1979.
- [2] B. Xie, Y. Liu, Y. Ding, Q. Zheng and Z. Xu, *Soft Matter* 7 (21), 10039-10047 (2011)
- [3] Y. Liu, Bo Xie, Z. Zhang, Q. Zheng and Z. Xu, *Journal of the Mechanics and Physics of Solids* (in the press)
- [4] B. Xie, Y. Liu and Z. Xu, *Mechanotunable networks of carbon nanostructures* (in preparation)