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PERSPECTIVES IN MECHANICS OF HETEROGENEOUS SOLIDS **

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ABSTRACT The Micro- and Nano-mechanics Working Group of the Chinese Society of Theoretical and Applied Mechanics organized a forum to discuss the perspectives, trends, and directions in mechanics of heterogeneous materials in January 2010. The international journal, Acta Mechanica Solida Sinica, is devoted to all fields of solid mechanics and relevant disciplines in science, technology, and engineering, with a balanced coverage on analytical, experimental, numerical and applied investigations. On the occasion of the 30^{th} anniversary of Acta Mechanica Solida Sinica, its editor-in-chief, Professor Q.S. Zheng invited some of the forum participants to review the state-of-the-art of mechanics of heterogeneous solids, with a particular emphasis on the recent research development results of Chinese scientists. Their reviews are organized into five research areas as reported in different sections of this paper. §I firstly brings in focus on micro- and nano-mechanics, with regards to several selective topics, including multiscale coupled models and computational methods, nanocrystal superlattices, surface effects, micromechanical damage mechanics, and microstructural evolution of metals and shape memory alloys. §II shows discussions on multifield coupled mechanical phenomena, e.g., multi-fields actuations of liquid crystal polymer networks, mechanical behavior of materials under radiations, and micromechanics of heterogeneous materials. In §III, we mainly address the multiscale mechanics of biological nanocomposites, biological adhesive surface mechanics, wetting and dewetting phenomena on microstructured solid surfaces. The phononic crystals and manipulation of elastic waves were elaborated in §IV. Finally, we conclude with a series of perspectives on solid mechanics. This review will set a primary goal of future science research and engineering application on solid mechanics with the effort of social and economic development.

KEY WORDS heterogeneous materials, smart materials, biological materials, multiscale mechanics, micro- and nano-mechanics, damage and fracture, constitutive relation, elastic wave, surface effects

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I. MICRO- AND NANO-MECHANICS

1.1. Multiscale Coupled Models and Algorithms at Micro and Nano Scales

Prediction of the mechanical properties and structural evolution of heterogeneous materials from nano, micro to macro scales is a difficult issue and involves multiscale and multiple field modeling. The high-order two-scale coupled models and the algorithms developed by Cui and coworkers[1–6] can be employed to simulate the physical and mechanical performances of composites, including stiffness, strength, and dynamically coupled thermo-mechanics behavior. Those models have been developed within the framework of macroscopic continuum theories and, therefore, cannot be used for some nano- or micro-sized structures.

Continuum theories and atomistic theories are two distinct classes of descriptions for material behavior. In continuum approaches, such quantities as stress, strain, and temperature are treated as continuous fields. By contrast, atomistic models explicitly acknowledge the discrete nature of matter. Therefore, various attempts have been done to construct multiscale coupled models and the algorithms, which can be divided into two classes. The first class is called 'mixed models' which use, concurrently or serially, both continuum and molecular dynamics (MD) methods. Typical examples are the quasicontinuum (QC) method[7,8], coarse-grained molecular dynamics (CGMD)[9], the bridging scale method[10], the heterogeneous multiscale method (HMM)[11]. The second class is generalized continuum models which are essentially non-local models of atomistic interactions developed by Eringen[12,13] and its variation[14]. Their difference is in the form of integral operator, and their commonness is the prior assumption of constitutive relation.

An alternative approach for generalizing continuum model is to derive continuum constitutive equations directly from atomistic model without any prior assumptions. The strain energy density function is directly obtained from the atoms, and then the stress-strain relationship is derived from the strain energy density function. The most representative approach is based on the Cauchy-Born rule[15,16]. Their basic technique is to approximate the strain energy density by using the Taylor series expansion of the atomistic interaction energy.

A new continuum-atomistic coupled model bypassing any empirical constitutive law and any local homogeneous assumption is constructed by making use of representative cells of atoms directly from transient MD results and the interaction potentials of the atoms[17]. In the model, the evolution equation is in a form the same as momentum conservation equation in continuum theory; its mass distribution is consistent with the continuum mass density; and its strain energy density is strictly derived from the nonlocal nature of atomistic interactions in representative cells of atoms. A stress-strain relationship is then derived from the variation of the energy density functional, invoking that the first Piola-Kirchhoff stress is the work conjugate to the deformation gradient. Essentially, the new continuum-atomistic coupled model is nonlocal and nonlinear. It is easy to reduce this model to high order strain-gradient models and Cauchy-Born model through Taylor series expansion.

As aforementioned, the Cauchy-Born rule or different implementations is the basis for several multiscale modeling algorithms, including the quasicontinuum method or the virtual internal bond method. A limitation of these methods is that they are largely limited to zero temperature studies, and that the technique is only applicable far from defects or large stress and strain gradients. An atomistic finite element method (AFEM) has been proposed recently[18], this approach might be implemented in building a multiscale numerical simulation framework for studying the mechanical behaviors of biological materials. One prominent merit is that AFEM is within a unified theoretical framework of continuum FEM, which makes combined AFEM/FEM a seamless and very efficient multiscale simulation method. Moreover, the AFEM is an order-N molecular simulation method, which is much faster than most other existing methods. This AFEM/FEM approach has been used to study the fracture behavior of carbon nanotube composites[19]. The mesoscopic method which connects the features of microscopic structure to the macroscopic properties and function is also a promising approach as part of the efforts bridging the scales from the atomistic to the macroscopic scales.

Up to now, nevertheless, a multiscale coupled model or algorithm that has been universally acknowledged is still not available. Some issues in multiscale coupled model and algorithm of micro-nano-scale computation are as follows:

Multiscale coupled models. It should hold the facticity in physics and mechanics to a certain extent. Untill now, are there any valid multiscale coupled models, which are reliable in theory, physics experiment or observation of original position?

Multiscale coupled computational methods. From nano, micro, meso to macro scales, the homogenization algorithm for constitutive parameters has been established. In contrast, the algorithm on physical and mechanical behaviors from nano, micro, meso to macro scales has many problems that deserve further study. For example, how can we treat the boundary conditions of smaller-scale sub-domain to transfer the information from larger-scale to smaller-scale? How to deal with the error of larger-scale computation so as not to be propagated to smaller-scale computation and how to avoid the ghost force in smaller-scale computation?

Effectiveness of multiscale coupled algorithms: a) Is the precision of computational results acceptable in nano-scale? b) Is computing cost and especially the computing time acceptable and sufferable? c) Can the multiscale computing process and its results be repeated by anybody in any case?

Verification of multiscale coupled simulations: a) Are there benchmark problems for examining new multiscale coupled model and algorithm? b) Are there the results of multiscale simulation in micro-nano-scale which have been verified by physical experiment and engineering survey?

1.2. Structures, Defects and Deformation in Nanocrystal Superlattices

Chemically synthesized nanocrystals such as PbS and CdSe can serve as artificial atoms and self-assemble into highly ordered structures called nanocrystal superlattices (NSs)[20]. The NSs not only exhibit quantum size effect, plasmon resonance and superparamagnetism[21], but also have mechanical properties comparable to strong plastics[22]. Thus these novel materials hold promise for many applications, including field-effect transistors, light-emitting devices, photodetectors and solar cells. A nanocrystal appears in NS as a composite particle consisting of a crystallite core covered by an organic ligand shell introduced in the synthetic process. The interaction between two particles is quite complicated, as it involves long-range attraction between the crystallites through van der Waals forces as well as short-range repulsion between the ligand shells which has both elastic and steric components[23]. In contrast to ordinary crystals, an outstanding nature of NSs is that the interparticle potential depends on the shape and size of the nanocrystals, implying that the properties of the NSs are highly tunable.

The shape and size dependence of interaction endows unusual structures and gives rise to a number of new mechanical phenomena of NSs. Of interest are the crystallographic structures and defects. High-resolution electron microscopy measurements showed that a mono-dispersed NS can be face-centered cubic (fcc), body-centered cubic (bcc) or hexagonal close-packed (hcp), depending on the size of nanocrystals[22]. The shape of a NS with small core size adopts the Wulff polyhedron so as to minimize the overall surface energy, as in the case of an ordinary crystal. However, when the size of the nanocrystal cores is large, the Wulff's rule is completely violated, accompanied by the presence of multiple twinning in NSs[24]. To date, the relationship between the crystallographic structure of a NS and the size of the core is still lacking, and the mechanism for multiple twinning formation as well as its influence on subsequent deformation of NSs remains to be explored. To answer these questions, a systematic theory of defects in NSs, as that for ordinary crystals, may be needed.

Recently, the mechanical properties of NSs have been studied with nanoindentation measurements[22]. A comparison of samples with different core sizes revealed a clear trend of decreasing stiffness with decreasing core sizes, opposite to the trend in colloidal crystals consisting of large polymer or silica spheres[25,26]. In addition, the moduli values for NSs are at least 6 orders of magnitude greater when compared to the colloidal crystals. These reflect the crucial effect of the ligand shells on the overall deformations. Though the short organic ligands are much reminiscent of a polymer matrix for they form a cohesive organic network surrounding the nanocrystal cores, the classic micromechanics theory of composite materials cannot be used directly to predict the mechanical behavior of NSs because it does not involve any size effect. A challenging problem is how to incorporate the role of the ligand shells in a continuum model.

The current insights into the mechanical behavior of NSs are very limited. This is extremely true for binary (two types of nanocrystals) or ternary (three types of nanocrystals) systems which possess more complicated periodic superstructures or even form dodecagonal quasicrystals[21]. The study in this field may lead to new defect and deformation theories which highlight the shape and size effects

of nanocrystal cores in NSs. Moreover, since the interparticle interaction, crystallographic structure, defect morphology and mechanical property of NSs are all tunable by simply adjusting the shape and size of the nanocrystals, they can also serve as an ideal prototype for the research of materials design.

1.3. Effects of Surface Stress and Surface Tension

The properties of heterogeneous materials have attracted much attention in recent years, e.g., the super-hydrophobicity of lotus leaf and the drag reduction of shark skin. Heterogeneous materials with microstructures and heterogeneous properties have been widely used in surface science, catalysis and nanotechnology areas and biological devices. However, it is difficult to describe the surface stress due to the complex heterogeneous surface profile. In order to overcome this difficulty, the effective surface stress and effective surface tension on the equivalent planar surface, which contain the effects of complex heterogeneous surface profile, have been defined. In the following, we will show several potential applications of effective surface stress (surface tension) in terms of the complex surface profiles.

Heat pipes use surface tension developed in fine porous wicks to circulate the working fluid. Porous metals prepared by dealloying have high porosity, high surface area, and good thermal conductivity which make them a great material for heat pipe wicks[27, 28]. However, the underlying transport mechanisms, such as fluid flow, phase change and heat transfer at interfaces are not well understood, nor is the potential of refining the capillary size to the nanoscale exploited in heat pipe technology. Thus, it remains a challenge to explore nano-(micro-) porous metals as heat pipe wicks and to clarify the underlying transport mechanisms.

Lithium ion batteries have become one of the most desirable power sources for many portable consumer applications and even for high power applications such as electric and hybrid electric vehicles. The performance of charge and discharge and the durability of the battery are key issues that people care. The lithium ion transport through inter- and intra-particles in porous electrodes induces the phase transformations in the solid phase of electrodes[29], and stresses generate due to intercalation and phase transformation processes in the electrode particles[30]. Thus, the volume of the electrode expands, and cracks or fractures occur in the material, which can lead to failure of the battery or even safety hazard. From the viewpoint of porous electrode[30], an increase in porosity of the electrode leads to a decrease in stress and an increase in conductivity, which improves both the mechanical life and the performance of the electrode. From the viewpoint of particle electrode, a decrease in the size of the active material particle decreases the magnitude of stress. Meanwhile, surface energy and surface stress significantly affect the magnitude and distribution of stress when the radius of the particle is at the nanometer scale[31]. Therefore, an electrode with smaller particles with optimum porosity for the desired application not only enhances the durability of the battery but also improves the performance of the battery.

1.4. Effects of Amorphous Evolution on the Behavior of Materials

Some advanced heterogeneous materials are often used under severe and harsh conditions, e.g., high temperature high radiation[32]. These courses inevitably induce atomic-scale defects, lattice disorders, and even amorphization in structure, affecting not only virtually the physical properties but also the mechanical performance of materials, which have attracted intensive experimental and theoretical effort.

Silicon carbide (SiC) as potential material applied to nuclear systems and space stations has been investigated to understand the disorder in amorphous SiC (α-SiC) existed in both chemical and topological structures. Chemical and short- and medium-range topological structures can be described in terms of chemical disorder χ ($\chi = N_{\mathrm{C-C}}/N_{\mathrm{C-Si}}$), C/Si centered tetrahedra and C/Si sublattices, respectively. Inspection of the evolvement of chemical and topological structures in melt-quenched α-SiC along with the quench rate proves the significant role of chemical disorder in topological structure. A tetrahedron-based model is proposed to describe the variation of short-range topological disorder as a function of chemical disorder[33].

Because chemical disorder can be applied to characterize the transition of crystalline to non-crystalline and to distinguish different amorphous SiC networks, it is reasonable to assess the dependence of mechanical properties on microstructure by examining the variation of mechanical properties as a function of chemical disorder. Molecular dynamics simulations of uniaxial tension and nanoindentation are performed on a series of SiC network with varying chemical disorder. Mechanical responses and prop-

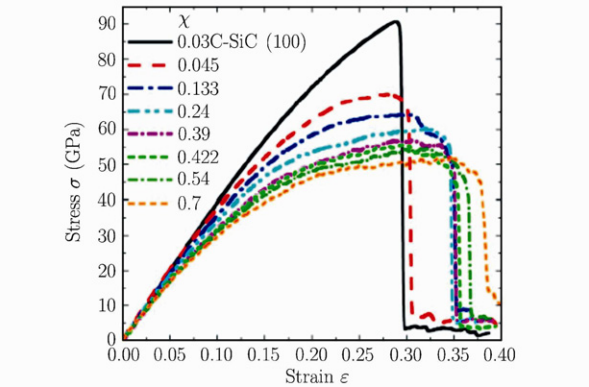


Fig. 1. Stress *vs*. strain curves for α-SiC samples with varying chemical disorder at a strain rate of 10^8 s^{-1}.

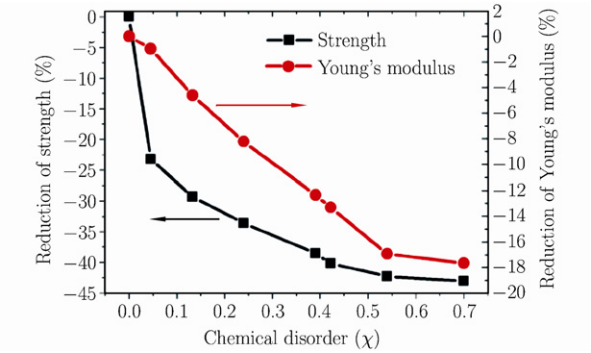


Fig. 2. Variations of Young's modulus and strength as a function of chemical disorder.

erties change from structure to structure, which can be understood in light of microscopic deformation mechanism[34].

Investigations of structural evolvements in tension and nanoindentation processes clearly indicate the crossover of deformation modes during the transition of crystalline to non-crystalline[35]. In tensile deformation, with increasing chemical disorder the homogeneous elastic elongation evolves into local plastic flow dominated by uncorrelated atomic slipping. Meanwhile the brittle fracture as a result of lattice instability evolves into nanoscale 'ductile' fracture preceded by the coalescence of nanocavities, as shown in Figs.1 and 2. The introduction of chemical disorder disrupts the continuity of atomic layers. The discontinuous atomic layer segments begin to decouple and deform independently, which is finally replaced by local plastic flow mediated by the adjustment of atomic arrangement in disordered clusters with increased chemical disorder.

1.5. Wetting, Electrowetting and Electro-Elasto-Capillarity

The moving contact line (MCL) problem as shown in Fig.3, a typical multiscale problem for wetting phenomenon, remains the focus of wide theoretical interest for mathematicians, physicists, chemists and engineers, in view of both its practical importance and a great variety of physical, chemical and mechanical factors operating on nanoscale, but influencing both macroscopic motion and interfacial shape far from the MCL. The biggest challenge of the MCL problem is the infinite energy dissipation at the three-phase point, which leads to the famous Huh & Scriven's paradox[36]: 'not even Herakles could sink a solid'. There are some possible mechanisms to solve this paradox, namely, the slip boundary, the diffuse layer between the liquid and vapor, and the precursor film, etc. Comparatively little attention has been paid previously to the MCL problem under electrowetting (EW). The two-dimensional (2D) propagation of the precursor film (PF)[37] and 1D water flow in nanotube[38] have drawn considerable attentions in recent years because of their unique transport properties.

The transport properties of PF, usually a single water molecular layer propagating ahead of the nominal contact line, in wetting and especially in EW were explored for the first time by using molecular dynamics (MD) and the molecular kinetic theory (MKT) in Ref.[37].

The propagation of PF obeyed the power law when droplet spreads (Fig.4(a)), supported by experiments[39] of about $R \sim t^{1/7}$. For the water molecules driven by the disjoining pressure on surface atoms separated by a distance λ with a frequency K_0, the advancing velocity is:

$$v = 2K_0\lambda \sinh \frac{w_V + w_P + w_S + w_E}{2\rho k_B T} \tag{1}$$

where ρ is the surface number density, k_B is the Boltzmann constant, T is the absolute temperature, $w_V+w_P+w_S+w_E$ is the driving work per unit area arising from the van der Waals interactions, the polar interactions, the different structure of PF and the electric field, respectively. When $w_V+w_P+w_S+w_E \ll \rho k_B T$, $v \sim (w_V + w_C + w_S + w_E)/\varsigma_0$, where $\varsigma_0 = \rho k_B T/(K_0\lambda)$ represents a friction coefficient. The power law $R \sim t^{n(E)}$ fitted well to the MD data in EW (Fig.4(b)). The steps were caused by the

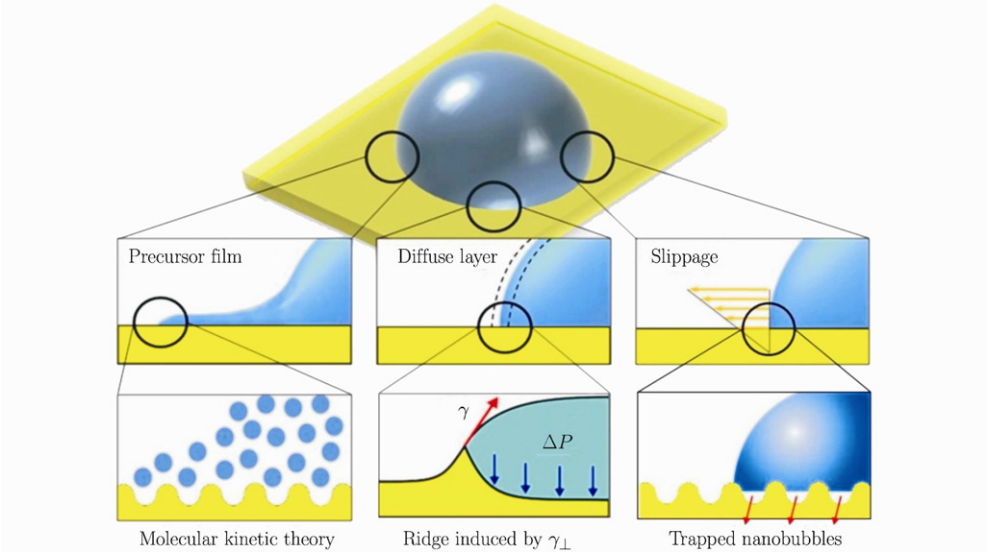


Fig. 3. Three possible multiscale mechanisms to solve the Huh & Scriven's paradox.

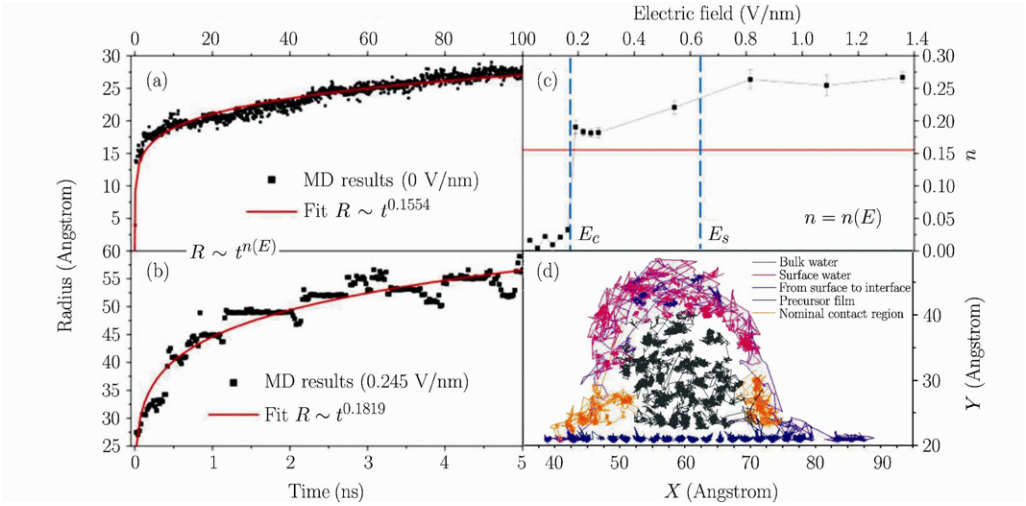


Fig. 4. The propagation of radius of PF with respect to time (See Ref.[37]) for (a) droplet spreading; (b) EW ($E = 0.245$ V/nm). (c) Change of n with E. The red line is $n = 0.1554$ when droplet spreads. (d) The path lines of water molecules belonging to different regions.

relaxation of water dipoles to electric field. A critical field $E_c(\sim 0.175$ V/nm) and a saturated field $E_s(\sim 0.625$ V/nm) were found in Fig.4(c), supported by experimental observations[40].

The path lines of water molecules in spreading were tracked in Fig.4(d). The new findings were: (1) The bulk water molecules, whose self-diffusion coefficient $D = 2.246 \times 10^{-5}$ cm^2/s[39], did random walk due to thermal energy k_BT. (2) The PF molecules had the lowest mobility, vibrating around one site with $D = 1.132 \times 10^{-5}$ cm^2/s in spreading (∼50.4% of bulk water), $D \sim 10^{-6}$ cm^2/s in EW (∼6% of bulk water). (3) The surface molecules had the highest mobility with $D = 7.354 \times 10^{-5}$ cm^2/s. Because they continuously and fast diffused ahead of PF and was then pinned by the surface, PF propagates fast with low energy dissipation. The path lines in EW validated this conclusion again. PF also has a unique 2D hydrogen-bond network inside itself. These results indicate that PF actually acts solid-like, no-slip and may be one of the answers to the Huh & Scriven's paradox, introducing atomic details to eliminate the infinite energy dissipation due to no-slip near the contact line.

To further explore the transport properties and show the importance of PF as an example, electro-elasto-capillarity (EEC) was simulated for the first time. First, since the radius of droplet is larger than

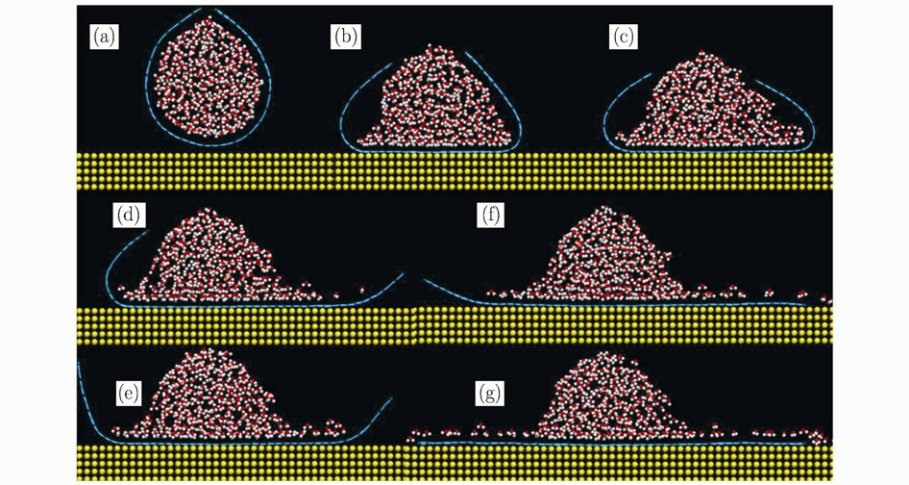


Fig. 5. The EEC process of a droplet on gold substrate[37].

the elasto-capillary length $L_{EC} = \sqrt{B/[(1+\cos\theta)\gamma]}$ (B: bending stiffness, θ: contact angle, γ: surface tension), the flexible graphene automatically wrapped the droplet. Then, this wrapped droplet was unwrapped under $E = 0.544$ V/nm along y-direction as shown in Fig.5. Because the propagation of PF is faster than the liquid above it, as well as the solid-like property of PF, PF pushes the graphene to unwrap with a force of the order of 1 nN/nm. So using the unique transport properties of PF, the EEC can be realized and used for the drug delivery at micro/nano scale.

1.6. Eshelby's Problem of Non-ellipsoidal Inclusions

Eshelby's problem of non-ellipsoidal inclusions has recently attracted a great attention because of its fundamental importance in mechanics of heterogeneous materials. For example, through transforming the analysis of disturbance stress field into algebraic operation problem, uniform Eshelby tensor of ellipsoidal inclusion is used to greatly facilitate the estimation of the effective properties of heterogeneous materials like composite material and crystal materials[42, 43].

Actually most inclusions (particles, holes, etc.) are non-ellipsoidal. Recently, it has been strictly proved that the strain field is no longer uniform within non-ellipsoidal inclusions, as Eshelby conjectured[44]. This conclusion made two obvious observations rather disturbing:

1. Eshelby tensor has been broadly used in the literature to deal with non-ellipsoidal inclusion problems without checking the validity of the underlying ellipsoidal approximation hypothesis.

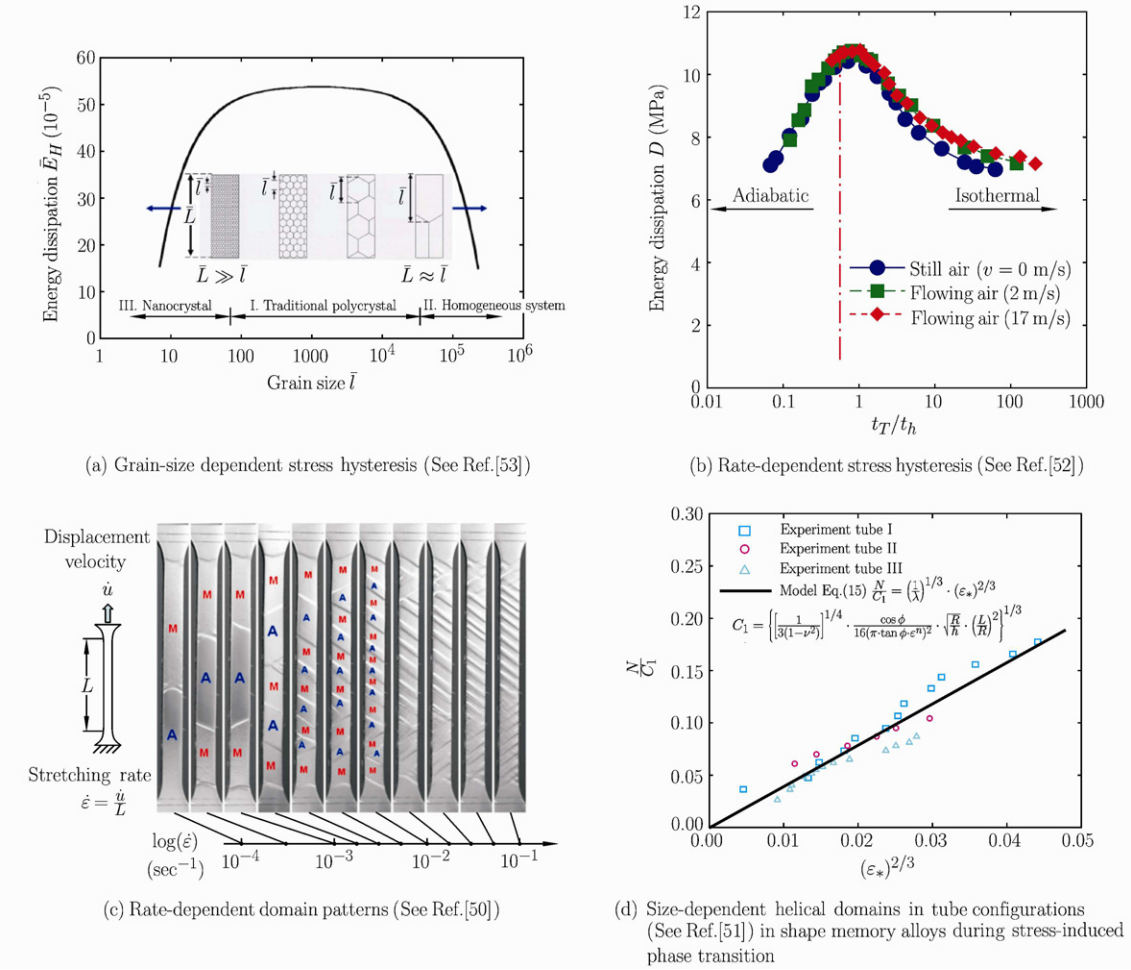
2. As a keystone of most of the existing micromechanics schemes, Eshelby's equivalent inclusion idea is frequently employed to estimate the effective properties of composites consisting of a matrix with non-ellipsoidal embedded inhomogeneities, though it holds only for an ellipsoidal inhomogeneity.

For two-dimensional Eshelby's problems of non-elliptical inclusions, Zheng et al.[45, 46] have reached the following results: (i) except for the elliptical approximation of convex inclusions, the elliptical approximation of non-convex inclusions may cause a large relative error and is in general inacceptable; (ii) replacing the generalized Eshelby tensor involved in various micromechanics schemes by the average Eshelby tensor of non-elliptical inhomogeneities is in general inadmissible. Similar results may be obtained for three-dimensional problems, that are undergoing to study.

II. EVOLUTION OF MICROSTURCTURE

2.1. Material Heterogeneity due to Non-Equilibrium Evolution

Basically, most processes in both material fabrication (e.g., solidification in casting of alloys, diffusion and displacive phase transition, high speed metal forming and cutting) and service such as various kinds of field-induced phase transition processes in structural and functional materials (either traditional or nano-structured) are intrinsically thermodynamic non-equilibrium. These processes involve, at one stage or another, different versions of material nonlinearity, instability and multi-field coupling at different



(a) Grain-size dependent stress hysteresis (See Ref.[53])

(b) Rate-dependent stress hysteresis (See Ref.[52])

(c) Rate-dependent domain patterns (See Ref.[50])

(d) Size-dependent helical domains in tube configurations (See Ref.[51]) in shape memory alloys during stress-induced phase transition

Fig. 6. Examples showing the roles of material instability, nonlinearity and multiscale coupling.

length and time scales, and constitute the main physical origins of material heterogeneity observed in various microstructure patterns and microstructure evolution under non-equilibrium conditions[47–49]. Typical examples include the phenomena of rate-dependent domain spacing in phase transition patterns of NiTi shape memory alloys[50–53] (see Fig.6) and the adiabatic shear bands in ductile metals, both of which are due to material nonlinearity and multiscale coupling.

Fundamental understanding and development of quantitative predictive models of the material heterogeneity and the resulting properties are of great interest for the control and development of new technologies for material synthesis. In addition to study the mechanical consequences of the above rich variety of micro- and sub-macro-scale heterogeneities, it is more important to understand how an initially macroscopic homogeneous material state becomes unstable under external driving, leading to macro- or micro-level emergent or self-organized structures (such as domain pattern formation and evolution). The research in this area is extremely rich and poses a great variety of challenge and opportunity for the solid mechanics community. The future research trend and topics include (but not limited to) the following:

(i) Physical origin of material heterogeneity

(ii) Formation of material heterogeneity under nonequilibrium condition

(iii) Instability and nonlinearity in the formation and evolution

(iv) Multi-physics (fields) coupled process and with multiscale (time and length scales) coupling and interaction

(v) Process involving multiple length scales, for example: grain-size dependent stress hysteresis in stress-induced phase transition and emergent length scale of deformation patterns.

2.2. Microstructure Theory of Metals

A polycrystal is an aggregate of tiny crystallites separated by grain boundaries. Since crystal lattices are often anisotropic, elastic and plastic properties of crystals differ in its orientation, which makes the elastic and plastic properties of the polycrystal depend on not only the chemical composition but also the crystallite orientation distribution. The orientation distribution of crystallites in the polycrystal can be described by the orientation distribution function (ODF)[54,55]. The ODF can be expanded under the Wigner D-bases. The expanded coefficients in the ODF are called the texture coefficients.

The early work on the elastic constitutive relation of polycrystals is due to Voigt and Reuss. The early study on polycrystalline plasticity is due to Sachs and Taylor. Under Sachs' model and Reuss' model, all crystallites in the polycrystal are assumed to have the same stress. For Voigt's model and Taylor's model, all crystallites in the polycrystal experience the same deformation. Man obtained an expression of constitutive relation for an orthorhombic aggregate of cubic crystallites[56]. Unlike Voigt's model and Reuss' model, the Man's expression is model independence.

The self-consistent method can ensure the traction continuity and the deformation compatibility among crystallites in a mean sense. Since Eshelby tensor is employed in the self-consistent method, the crystalline mean shape of the polycrystal is elliptic. Huang et al. employed the crystalline shape function to derive the elastic constitutive relation of the polycrystal with the effect of crystalline mean shapes[57]. Man and Huang et al. derived the constitutive relation of a weakly-textured orthorhombic aggregate of cubic crystallites with effects of microstructure and initial stress[58,59]. By means of the constitutive relation, electromagnetic transducers and piezoelectric transducers have been used to measure the microstructure and initial stress of sheet metals online.

Hill proved that Voigt's approximation and Reuss' approximation are an upper bound and a lower bound of elastic constitutive relation, respectively. For isotropic aggregates of cubic crystallites, Hashin and Shtrikman derived lower and upper bounds for the effective stiffness tensor, which are tighter than the lower and upper bounds provided by the Reuss model and Voigt model, respectively. Huang and Man[60] provide lower and upper bounds of the effective stiffness tensor for weakly-textured aggregates of cubic crystallites.

Man[61] and Man and Huang[62] proposed the expressions of the yield function and r-value on a weakly-textured orthorhombic aggregate of cubic crystallites which include the effects of the ODF up to terms linear in the texture coefficients. The r-value of a sheet metal is a measure of plastic anisotropy frequently used for prediction of performance in deep-drawing.

2.3. Micromechanical Damage Mechanics

The ductility, strength and fatigue life of materials are always a topic for which mechanical and material engineers show great concern. It has already been realized that the mechanical properties of materials are closely related to their microstructures, and great effort has been made on it in the past decades, of which much effort was made on the effect of the characteristic size of micro/meso structure on the strength of the materials. The studies of damage mechanics have achieved significant progress and contributed to the developments of engineering and technology[63].

Recently, Peng et al.[64] investigated the ductility, strength and fatigue life of lamellar two-phase materials from the viewpoint of microstructure damage. Taking pearlitic steel as an example, it is composed of numerous randomly orientated colonies, and each colony is further composed of many alternatively arranged parallel fine lamellas of ferrite and cementite. It possesses excellent mechanical properties, such as high rupture strength, good resistance against wear, and long fatigue life, etc.[65–68]. Systematic experiments on the mechanical properties of pearlitic steel PD_3 of different interlamellar

Table 1. **Mechanical properties of pearlitic steels with different interlamellar spacing**

Material states	h (nm)	σ_b (MPa)	δ (%)	N (10^6 cycles)
Hot-rolled	254	1100	7	1.30
On-line quenched	136	1260	15	3.18

spacing h but similar size of pearlitic colonies were made by Sheng et al.[66,67], and the main results are shown in Table 1. It was found that the ultimate strength σ_b, elongation ratio δ and contact fatigue life N increase remarkably with decreasing h (regarded as the most important characteristic size of its microstructure).

The size effect on the strength, ductility and fatigue life of pearlitic steel was investigated by Peng et al.[64] with a microstructure-damage analysis and a micro–macro approach. Assuming different patterns of microdefects in different phases in the RVE, as shown in Fig.7, a unified damage evolution law was derived as

$$\Delta d_k = \lambda_k \boldsymbol{\sigma}_k : (\Delta \boldsymbol{\varepsilon}_k - \Delta \boldsymbol{\varepsilon}_k^e) h \tag{2}$$

with λ_k a material constant determined by the volume fraction, the energy release rate and the fraction of the energy dissipated on the damage in the phase k. It indicates that damage develops slower in the material with smaller h, accounting for why the material with smaller h possesses higher rupture strength, better ductility and longer fatigue life.

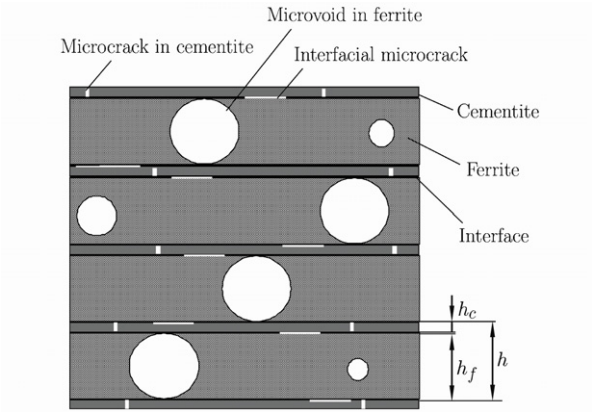


Fig. 7. RVE of pearlitic colony with different patterns of microdefects.

The damage as well as its evolution was embedded in the constitutive model for each individual phase. The description for the elastoplastic and damage behavior of a single colony was then derived, taking into account the interaction between phases. The constitutive model for the lamellar two-phase material was finally obtained with the self-consistent scheme, taking into account the interaction between colonies.

The responses of the pearlitic steel with different h were analyzed. Figure 8 shows that the material with smaller h possesses batter strength and ductility, well replicating the experimental results (Table 1). Figure 9 shows the ratcheting of the materials subjected to asymmetric tension/compression cycling, which implies that the material with smaller h possesses longer fatigue life.

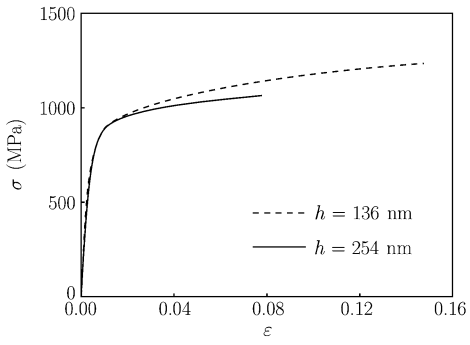


Fig. 8. Size-effect on strength and ductility.

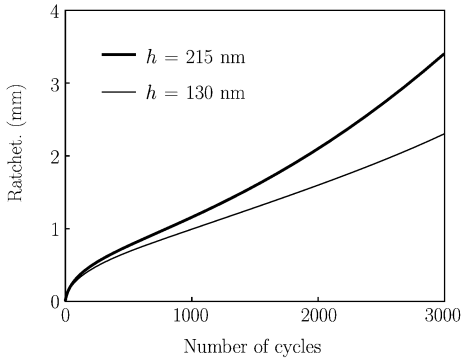


Fig. 9. Ratcheting under asymmetrical cyclic loading.

Another class of typical damage mechanisms at meso scale is the nucleation, growth and coalescence of microcracks. Based on the concept of orientation domain of microcrack growth (DMG), Yu and Feng[69] established a micromechanics damage model for microcrack-weakened quasi-brittle solids. This model accounted for the effects of various damage mechanisms, e.g., stable and unstable propagation of microcracks under tension, frictional sliding and kinking of microcracks under compression. In addition, Feng et al.[70] suggested a micromechanics method for calculating the interaction of microcracks of a large number and/or a high density. They calculated the effective elastic moduli of elastic solids containing microcracks with random or aligned orientations and studied the size dependence of failure of brittle materials due to the stochastic nature of disordered microcracks. Ren et al.[71, 72] extended the above work to the case of elliptic crack, and applied it to the analyses of rock-like materials subjected to triaxial compression and coupled tension and shear loadings. Ma et al.[73] examined the influences of such factors as non-uniform dispersion of microcracks on the effective elastic moduli and strengths of microcracked solids. They also adopted this method to calculate the strength of a microcracked beam subjected to bending and extended the above numerical method to study the coalescence of microcracks and the associated fracture process of elastic solids containing many microcracks.

Issues remained:

(i) What is the real mechanism of the size effect? Besides the proposed approach, the traditional Hall-Petch relationship, which can be related to the packing of dislocations, has also been extended to sub-micron and nanometer size of grains. The plastic strain gradient theories can also describe size effect, but the physics background and determination of the adopted characteristic length need further investigation, especially when the characteristic size of materials reduces to sub-micron or nanometer scale.

(ii) During the development of multiscale modeling, 'there is a particular shortage of dedicated experiments which can be used to gain physical insight and to interact with model developments', because there are difficulties to separate each phase from the material without changing its characteristic size, its in-situ residual stress and strain, and its internal structure, for instance, microdefect states and evolutions, and in turn, the realistic independent constitutive behavior of each individual phase. Although nano-indentation may provide some information of some individual phase at constrained states, the inverse approaches as well as their effectiveness and uniqueness of results need further investigation.

(iii) For some multi-phase materials, e.g., nano-grained NiTi shape memory alloys, the constitutive responses under different states of stress (e.g., pure tension, pure compression or pure shear) are distinctly different, which do not following any existing equivalent rules[74, 75]. Although the formulation from transformation kinetics of martensite variants could partly account for the differences, it failed to cover the marked differences, even between the response under pure tension and that under torsion. Distinct difference between surface morphologies of specimens under different states of stress was observed[74, 75], implying the difference in microstructure, with which, an microstructure based approach has been developed to account for such difference[76]. However, more efforts are needed for the in-depth investigation.

(iv) Multiscale modeling of materials of nanometer scale microstructure. Nano-multilayered coatings composed of two different metallic-nitrides is a kind of promising coatings with extremely high hardness, in which the thickness of each layer is only several nanometers. It was found that the hardness of nano multilayered TiN/VN can reach about 56 GPa[77–79], much larger than that of any of its host constituents. However, the mechanism for such excellent property remains unclear, though some hypotheses, such as lattice mismatch, modular difference, coherently epitaxial growth, Hall-petch effect, etc. have already been suggested. In order to gain an insight into the constitutive behavior of such nano-multilayered coatings, an multiscale approach is necessary, which may cover atomistic, quantum mechanical, meso- and macroscopic scales. Taking TiN/VN nano-multilayered coating as an example, through a thorough analysis of the electronic property and bonding configuration at the TiN(111)/VN(111) interface with atomistic first-principles calculations, the electronic states near the interface were characterized, the interfacial bonds are found to be mainly ionic, and potential function of the newly formed interfacial bonds and the elastic properties of the host constituents were obtained[80]. The mechanical properties of the coating and their dependence on the characteristic size of the microstructure are to be investigated with an MD approach, based on which, practical macroscopic model should be formulated for engineering

application. This approach may encompass the knowledge that can hardly be obtained directly in experiment, and provide information for the design and modelinig of such kind of materials.

(v) Microstructure based multiscale modeling for the properties of heterogeneous materials is a key interface between materials science and mechanics. How can mechanics use more quantitative materials information in modeling and how can materials science and physics push mechanics into greater fidelity and reality with regard to mechanisms? What are the tradeoffs?

III. MECHANICS FOR MULTI-FIELD COUPLED BEHAVIOR

3.1. Multi-Fields Actuations of Liquid Crystal Polymer Networks

Smart materials are distinguished by their ability to deform and consequently to generate mechanical energy under external stimuli other than mechanical means. Typical examples are shape memory alloys (such as TiNi) by thermal actuation, ferroelectric ceramics (e.g. $BaTiO_3$, PZT and PLZT) by electric field, and giant magnetostrictive materials by magnetic field. These materials have to be well designed to be activated by proper fields.

Liquid crystal polymer networks (LCNs) are cross-linked polymer materials with liquid crystal (LC) molecules in their main or/and side chains[81]. Since the LC molecules can be easily activated by thermal, electric, magnetic, chemical and optical fields, LCNs are an ideal material system that can be designed as smart materials with multi-fields actuations.

The possible unusual mechanical behavior of LCNs was firstly predicted by De Gennes[82]. The nonlinear mechanical behavior called soft and semi soft elasticity was brought to light for the mechanical community by the review of Warner[83] and attracted since then quite a few interests in modeling and simulations[84–87]. The unique actuation by UV light of specially designed LCN systems[88,89] opened a new perspective to build remote controllable actuators and tetherless micro machines[90]. The opto-mechanical effect is a consequence of three processes occurred in different time and space scales[87]. The first process is the photoisomerization of certain photochromic molecules, e.g. Azobenzene, followed by different isomers triggering the collective reorientation of the LC molecules so to induce a LC phase transition. In the final process stage, macroscopic deformation of the polymer network is induced by the reoriented LC molecules which are linked to the network through flexible spacers. Ferroelectric and antiferroelectric LCNs are reported with excellent electric-mechanical couplings[91]. Mechanical-optic effects have been studied with such promising applications as smart optic devices[92].

As a typical soft material, the effect of entropy has to be considered in order to understand the behavior of LCNs. The change of entropy is related to a change of the ordering of loosely bounding molecule systems such as LC molecules, polymer molecules, etc. This costs very little energy and the change of ordering in one space scale can be easily and often rather quickly transferred to other scales. Thus, the entropy is the key of the interesting phenomenon observed in LCNs. The present modeling is mostly phenomenological by introducing some internal variables to describe the molecule structures and to insert them into the free energy function of the materials through ad hoc assumptions. Such models can simulate quite a lot of interesting phenomena observed in LCNs. However, a model that can help to clarify the characteristics of the processes in different scales is very useful to better design of more effective materials. Future work should focus on multiscale models based at least partly on statistical calculations of the entropy. Bottom up models are still too costly for such complicated systems but can give very useful information for the multi processes occurred in different space and time scales.

3.2. Mechanics of Materials under Radiations

Radiations are particularly strong in space and in nuclear reactors. The mechanical behavior of materials in a strong radioactive environment is generally very different from that in normal conditions. With the number of nuclear power plant built in China increasing, the safety and longevity of the power plants become a serious issue for mechanics research. One of the key points is to understand and to model the irradiation effects of materials. From their applications, materials in nuclear engineering and technology may be divided into two main categories: nuclear fuels and nuclear materials. Nuclear fuels are materials with radioactivity and are used as fuels to produce energy in nuclear reactors. Typical examples are UO_2 used in most commerce power plants as the fuel elements. Nuclear materials are all other materials used in nuclear environments such as stainless steels, zirconium and zircaloy. Zircaloy

is widely used as the cladding of nuclear fuels and thus is exposed to most severe radiation conditions. Various types of stainless steels are used as structure materials inside nuclear reactors.

Nuclear fuels and materials behave very differently. The following issues have to be considered:

(i) Very severe operation conditions of high temperature, high pressure and strong corrosion. Thus, thermal stress is generally very large[93] and the corrosion fatigue has to be considered together with the stress fatigue.

(ii) Evolution of material properties due to irradiation. Almost all mechanical properties of materials such as the elastic modulus, strength and extensibility, vary significantly when subject to irradiation of energetic particles. Thus, the constitutive equations have to be taken as time and space dependent. A more feasible way is to introduce an internal variable into the constitutive equations to represent the radiation damage[94]. Ductile materials can transform to behave very brittle after irradiation and thus change the fracture characteristics as well.

(iii) Effect of new materials produced by nuclear and chemical reactions. For example, inert gases such as Helium are produced inside nuclear fuels due to nuclear reactions. The presence of the fission gas affects the mechanical properties of the fuel materials very strongly[93].

3.3. Micromechanics of Heterogeneous Materials

The art of material design is built upon reliable quantitative relations between the microstructure and macroscopic behavior of materials. To establish such relations, we usually search for a homogeneous material to replace a heterogeneous one so that the two are deemed to have similar (if not the same) behavior. For some macroscopic quantities (e.g., like stiffness, conductivity and thermal expansion) which are insensitive to microstructure arrangement, classic micromechanics methods can provide reasonably accurate predictions. For other macroscopic quantities such as strength, plasticity and damage, however, they are sensitive to the actual detailed configuration of microstructures and the micromechanical methods usually fail to give a precise prediction[95]. The reason originates from the framework of micromechanics itself. Because the macroscopic quantity is defined by spatial or ensemble average of the local corresponding one, this needs the microstructure to be statistically homogeneous. For composites with evolving microstructure under external loading, e.g., shear band formation due to plasticity and macro-crack formation by overwhelming small ones, the statistical homogeneity is lost. Therefore, it is a field to be explored as to how to put more microstructure information into micromechanics models while retaining its analytical nature.

When the microstructure size is comparable to the macroscopic one, coupling between micro- and macro-levels becomes more pronounced, giving rise to various size effects[96]. It is well accepted that high order continuum models can describe this size effect in a phenomenological way. However, the intrinsic length scales introduced into the high order continuum models are still waiting for a clear and decisive explanation from micromechanics and experiment points of view. Some effects have been made by considering the nonlocal effect of composite materials[97] or by imposing particular boundary conditions over a representative volume element[98–100]. Indeed, the intrinsic length scales are related to the local material microstructure and its spatial distribution. However, work along this vein is far from complete. More effort is necessary to derive these length scales from local information in a more general context. Most experimental investigations on the size effect are conducted in an indirect manner. More simple while decisive experiments are needed to explore the origin of size effects.

As a kind of energy propagation, wave propagation phenomenon has an important impact on engineering applications, e.g., stealth technology, energy harvesting and noise isolation. By tailoring the microstructure, we can control wave propagation in a desired way. The recent advances in metamaterials (composites with unusual macroscopic property due to local resonance) provide an unprecedented way for wave control[101, 102]. For such materials with the feature of local resonance, the wave length is usually comparable to the microstructure size necessary for homogenization and nonlocal effect may become important[103]. It is thus necessary to develop a dynamic micromechanics tool for the design of metamaterials.

IV. MECHANICS AND BIOMIMETICS OF BIOLOGICAL MATERIALS

Through many millions of years of evolution, living organisms have developed various materials with superior mechanical properties to achieve different biological functions. These materials exhibit struc-

tural hierarchy from nano, micro to macro scales. For examples, bones, teeth, and shells are hierarchical biological nanocomposites with nanostructures made of mineral crystals and protein. Wood and silks of spiders and cocoons have similar structural hierarchy with nanostructures out of crystalline and amorphous bio-polymers. While different biological nanocomposites differ widely in their microstructures and can dynamically adapt to changing environment. They exhibit convergent evolution in the form of a network of interspersed hard and soft phases at the nanostructure level; the hard phase provides a basic structural scaffold for mechanical stability and stiffness, while the soft phase absorbs mechanical energy and provides toughness, support, and damage buffer for the composite[104–106].

The hierarchical structure of biological materials is assumed to have gradually developed and improved over the long course of natural evolution to maximize the chance of survival of various living creatures. In this evolution, mechanical forces have no doubt played critical roles in shaping biological systems into what they become today. Inspired by the superior mechanical properties of the biological materials, many intensive researches have been conducted in the past few decades to pursue the basic mechanisms and principles behind the design of the hierarchical structures from the nanoscale. Brief review on recent progress on these studies will be given in the following by categorized by the biological nanocomposites, the biological adhesive surfaces and the biological water-repellent surfaces.

4.1. Biological Nanocomposites

Regarding the biological nanocomposites, significant progresses have been made in understanding of high toughness of biological nanocomposites from various points of view including their hierarchical structures, the mechanical properties of protein on stress redistribution and energy dissipation, protein-mineral interface roughness and reduction of stress concentration at a crack tip, mineral bridges on the surface of mineral platelets[107]. A tension-shear chain (TSC) model was suggested to capture the essential features of load transfer and deformation in the protein-mineral nanostructure of the bone-like materials[104]. This simple model has been used to address why the elementary structure of biocomposites is designed on the nanometer length scale, suggesting a flaw tolerance concept for the design of strong materials. Other progress includes the strength of protein-mineral interface, and how the toughness, the elastic stability and other mechanical properties are related to the nanostructure[105].

Nacre, a type of natural biomineralized materials, is well known for its excellent mechanical properties generated by its unique microarchitecture, in particular, its high toughness, and it has, thus, become an attractive target for the microstructural design of toughened synthetic ceramics. However, the understanding of the physical mechanisms underlying the mechanical behaviors of nacre is still elusive. Song et al.[107] confirmed the existence of nanosized mineral bridges in the organic matrix layers of nacre and proposed a distribution law of the mineral bridges. They demonstrated that the mineral bridges can increase the strength of the organic matrix layers by about 10 times. Recently, the effect of a negative Poisson ratio is experimentally revealed in the tension deformation of a nacre sample[108]. This effect can increase the volume strain energy per unit volume by 1100% and, simultaneously, decrease the deformation strain energy per unit volume by about 44%, so that it effectively enhances the deformation capacity by about 1 order of magnitude in the tension of the material. It also shows that the physical mechanisms producing the effect are attributed to the climbing on one another of the nanostructures in the natural material, which provides a guide to the design of synthetic toughening composites.

Dai and Yang[109] studied the macro/micro-structures and mechanical properties of the elytra of beetles. Their SEM images show the similar geometric structure in transverse and longitudinal sections and multilayer—dense epicuticle and exocuticle, followed by bridge piers with a helix structured fibers, which connect the exocuticle to the endodermis, and form an ellipse empty to reduce the structure weight. The elastic modulus and the hardness are topologically distributed and the mechanical parameters of fresh elytra are much higher than those of dried elytra. The tensile strength of the fresh biological material is twice that of dried samples, but there is no clear difference between the data in lateral and longitudinal directions[110]. Coupling forces measured are 6.5 to 160 times of beetles' bodyweight, which makes the scutellum very important in controlling the open and close of the elytra[111]. The results provide a biological template to inspire lightweight structure design for aerospace engineering.

The mouthparts of female mosquitoes have evolved to form a special proboscis, a natural biomicroelectromechanical system (BMEMS). Kong and Wu[112] shows that the mosquito proboscis consists of a small bundle of long, tapering, feeding stylets that are collectively called the fascicle, and a large

scaly outer lower lip called the labium. During blood feeding, only the fascicle penetrates the skin while the labium buckles back to remain on the surface of the skin. The mosquito does not directly pierce its fascicle into victim's skin, instead, uses the maxillae as a variable frequency micro-saw with nanosharp teeth to advance into the skin tissue. This elegant BMEMS enables the mosquito to insert its feeding fascicle into human skin using an exceedingly small force (tens of micro-Newtons).

Biological protein material such as silkworm silk, spider silk, keratinous horn and protein matrix in nacre, plays important roles in providing mechanical functions to biological systems due to its superior mechanical properties. Zhao et al.[113, 114] studied hierarchical structure and mechanical properties of silkworm cocoons and silks. A cocoon is a natural polymeric composite shell made of a single continuous silk strand with a length in the range of 1000-1500 m. Coated by a layer of sericin, a raw silk fiber consists of two fibroin brins bonded together. Interestingly, the elastic modulus, strength and thermo-mechanical parameters of a cocoon vary along the thickness direction of a cocoon in an apt manner, further enhancing its ability to resist possible attacks from the outside. Moreover, their experimental results and statistical analysis on the properties of silkworm silk showed that the diameter and mechanical properties of silk have significant variabilities at both the intraspecific and intraindividual levels, and distinct size effects were observed in the properties of silkworm silk. In addition, Li et al.[115] studied another type of protein materials, keratinous horn shell. The microstructure and properties of keratinous horn shell interestingly show that, on one hand, the cattle horn sheath keratin has a laminar structure consisting of flattened, curved dead keratinfilled epithelial cells; on the other hand, the horn sheath exhibits very high fracture resistance, which is critical for maintaining its biological functions. Its mean K_{IC} varies from 2.56 MPa $\mathrm{m}^{1/2}$ at 19% water content to 4.76 MPa $\mathrm{m}^{1/2}$ at 8% water content. Somewhat surprisingly, the K_{IC} of the horn sheath is of the same order as that of bone and abalone sheath, and it exceeds those of the enamel and dentin in teeth.

Recently, Zhao et al.[116] compared the microstructure and mechanical properties of *Haliotis discus hannai Ino* (abalone shell) and *Hemifusus tuba* conch shell. Their results indicate that the size of inorganic substance is not a dominant factor to improve strength, while both proteins in shells and the microstructure of inorganic matter also play important roles. Further, Zhang et al.[117] compared the microstructures and mechanical properties of honeybee and silkworm silks.

The Possion's ratio of the soft matrix in biocomposites is usually very close to 0.5, which implies the bulk-incompressibility. Recently, Liu et al.[118] found the Possion's ratio can play an important role in compression resistance of biocomposites, and the incompressible soft matrix can convert deformation mode like a hydraulic machine. Moreover, when the Possion's ratio approaches 0.5, many well-known estimations on stiffness might be improper[119].

4.2. Biological Water-Repellent Surfaces

Nature has also evolved various forms of hierarchical surface structures. For example, the adhesive hairy structures on the foot of flies, spiders, and geckos, which allow for instance the gecko to adhere to and move along freely on the vertical wall and ceilings; the superhydrophobic anti-adhesive structures of plant leafs and the hairy structures of insects, which allow the plant leaves to be highly water-repellent and insects like water strider to walk on water via surface tension. These biological surface structures are also hierarchically structured from nanoscale up to macroscopic scale.

Classical theory indicates that large pressure drops are required to cause fluid flow in micro- and nano-channels. The motivation for exploring methods to decrease the required pumping power in microfluidic applications is thus considerable[120]. One promising avenue is the so-called superhydrophobic surfaces, which were initially inspired by the unique water-repellent properties of the lotus leaf and can be employed to produce drag reduction in both laminar and turbulent flows, reducing the viscous dissipation in the microfluidic devices. Microfabrication techniques permit the manufacture of such patterned surfaces as posts, cavities, or others, over which the liquid surface remains suspended due to the effect of surface tension. Water will slip on the shear-free air-water interface supported. A slip length over 10∼100 μm can be achieved, much larger than the mean free path predicted first by Maxwell. To date, although the performance trends are generally understood, only a small subset of possible surface geometries has been investigated. There must be critical hydro-pressure that can be supported before the air-water interface is driven into the space between the surface roughness. Surface optimization must be carried

out to develop surfaces capable of maintaining an interface and performance under large hydro-pressures if the superhydrophobic surface is to become mainstream[121].

Two widely adopted models that connect surface roughness and hydrophobicity are Wenzel's model and Cassie-Baxter model. In the so-called Wenzel state, water forms seamless contact with a surface and the contact angle changes with the surface roughness. In contrast, the Cassie state refers to water forming incomplete contact with a rough surface with air trapped between the liquid and solid. Experimental and theoretical studies have shown that the Cassie state is more reasonable for the Lotus effect in view of its incomplete contact and relatively weak adhesion with water droplets. A number of studies have attempted to investigate the stability of the Cassie state and the transition between the Cassie state and the Wenzel state. Recently, Zheng and his colleagues performed a rigorous study on the stability, metastability and instability of the Cassie and Wenzel states with periodic micropillars model[122], revealed the structural stability effects on self-assembling of carbon nanotube films[123] and two-scale lotus' structural surfaces[124]. They found through theoretical and experimental studies that scaling-down roughness into the micro-submicron range is a unique and elegant strategy to not only achieve superhydrophobicity but also to increase its stability against environmental disturbances[125]. The quantitative understanding of the question why the biological surfaces are hierarchically structured from nanoscale was recently pursued[124, 126–128].

Wu et al.[129] studied the floating mechanics of mosquito and the micronanostructured surfaces of mosquito's legs. They found that the mosquito's legs are covered by numerous scales consisting of the uniform microscale longitudinal ridges and nanoscale cross-ribs. Such special hierarchical delicate structures on the insect leg surface give a water contact angle of $\sim 153^\circ$ and give a surprising higher water-supporting ability. Experiments showed that a single leg of the mosquito gives rise to a water-supporting force of about 23 times as large as its body weight, compared with a water strider's leg giving a water-supporting force of about 15 times as large as its body weight[130].

4.3. Biological Adhesive Surfaces

Adhesion systems in biology, including those of gecko and many insects, have attracted significant attention in recent years. In studying of the gecko adhesion system, Artz et al.[131] suggested a contact splitting concept to explain the mechanism of gecko achieving high adhesion ability through hairy surface structure. Later, the nanometer size of the most terminal hairy structures of gecko, was found to be responsible for allowing the hairy structures to achieve maximum adhesion strength and become insensitive to variations in the tip shape[132] and crack-like adhesion flaws in the contact regions. Gao and Yao[132] showed that structural hierarchy plays a key role in robust adhesion: it allows the work of adhesion to be exponentially enhanced with each added level of hierarchy. Reversible adhesion has been studied at the level of a single seta of gecko. Gao and Chen[133] , Chen and Gao[134, 135] found that the asymmetrical alignment of seta allows the pull-off force to vary strongly with the direction of pulling. More recently, Chen et al.[136] generalized the adhesive contact model by accounting for the effects of elastic anisotropy. Their finding provides a feasible explanation of why most biological adhesive tissues are anisotropic. Chen et al.[137] developed the adhesive contact model for a typical bio-mimetic graded elastic material, whose Young's modulus varies with depth according to a power law. Closed-form analytical solutions were established for the critical force, the critical radius of contact area and the critical interfacial stress at pull-off. To study the size effects and micro-mechanisms in bio-adhesion, Chen et al.[138] studied the adhesive strength for a single fiber and fibrillar structure. They found a limited region for the radius of a viscoelastic fiber under which the normal and tangential contact interface strength would achieve the theoretical one, and the total adhesion strength for a fibrillar structure could be improved by tuning its geometrical parameters. Peng et al.[139] proposed a peeling model to analyze the peeling properties of bio-mimetic nano-films for understanding the micro-adhesion mechanisms of biological systems, e.g., gecko.

In contrast to the dry adhesion via van der Waals force, the 'wet adhesion' uses the capillary force via liquid bridges between the biological surfaces and the substrate, which has been widely adopted by many insects and animals from beetles, flies, spiders, to geckos/lizards and tree frogs. Recent experiments evidenced the significant contributions of capillary force to the adhesion of geckos. The presence of water also strongly affects the adhesion of geckos by measuring the adhesion force. Therefore, geckos can use both van der Waals force and capillary force to enhance their adhesion. In comparison with

van der Waals force, the capillary force is a long range force and can take effect at a larger scale.

4.4. Perspectives

The mechanical principles of biological systems can play an important role in helping address some of the major challenges in materials sciences and engineering. Understanding these principles requires systematic studies on how biological structures adapt to internal and external forces. A strong interdisciplinary approach is needed to extract the basic concepts and principles from the apparent complexity of nature. Here we will discuss some aspects of the challenging fields as follows.

4.4.1. Mechanical principles in design of biological hierarchical materials

The key for the remarkable properties is the complex hierarchical structure of the natural materials built from nanoscale. One of the important objectives of materials sciences and engineering has been to understand the relationships between microstructure of materials and their macroscopic mechanical properties. From this point of view, knowledge about the structures and mechanical properties of biological systems are significant to materials research. In principle, living organisms should strive for efficient use of materials through optimized structure design; they should not waste valuable energy resources on developing and maintaining structures or materials which either function inefficiently or have no function at all. Structures that function abnormally or inefficiently are gradually eliminated or replaced by more efficient ones during the course of evolution. Those that are found to work are continuously optimized, allowing the organisms to adapt better to the environment. These optimizations are generally regarded as strong hints that some properties important for the survival of an organism have been optimized.

Nano- and micro-technologies promise to enable mankind to eventually design materials using a bottom-up approach, i.e. to construct multi-functional and hierarchical material systems by tailor-designing structures from atomic scale and up. Currently, there is no theoretical basis on how to design a hierarchical material system to achieve a particular set of functions. The efforts aimed to extract the basic mechanical principles of multiscale and multifunctional materials design are in the frontier of materials sciences and engineering. It is hoped that this paper could stimulate some further interests in this emerging research field.

4.4.2. Multiscale theoretical and numerical methods

From a theoretical viewpoint, major challenges are the development of new materials theories that overcome the barrier that currently separates the scales to fully understand multiscale or cross-scale interactions. Future studies should address the questions, e.g., how to connect the microstructures at different scales and the macroscopic mechanical properties of the materials? How does Nature design materials that are lightweight and yet tough and robust and can serve multiple objectives? What are the roles of different kinds of forces, such as the van der Waals force, Casimir force, capillary force, electronic static force, etc., at different length scales? How do universality and diversity integrate into biological structures? What will and can our impact be, in a long perspective, in understanding fundamental biology and developing biomimicking materials?

The presence of hierarchical structures calls for new paradigms in thinking about the structure-property relationship. Predicting the properties and behaviors of materials by computer simulation from a fundamental perspective has long been a vision of computational material scientists. The key to achieving this goal is utilizing hierarchies of paradigms that connect macrosystems to the basic building blocks. Such approaches should build mutual 'talk' between different spatial and time scales, and take into account the interaction of different phases, e.g., the organic and inorganic phases, at their interface, by developing unified frame work including the continuum approaches, the molecular dynamics simulation methods (e.g., the atomistic and the coarse-grained) featured by different force fields and quantum mechanics simulation method, to bridge different spatial and time scales.

4.4.3. Measurement and characterization of the biological materials at different scales

Now experimental techniques have gained unparalleled accuracy in both length and time scales, as reflected in development and utilization of Atomic Force Microscope (AFM), optical tweezers or nanoindentation to analyze biological materials. At the same time, modeling and simulation have evolved into predictive tools that complement experimental analyses. For studying of the biological hierarchical material, it is desirable to develop tools that can access the microstructures of materials

starting from the smallest scale, e.g., the atomistic scale, to reach all the way up to macroscopic scales, by characterizing structural features at each scale.

However, there are many challenges that make developing these experimental tools extremely difficult. For example, bond energies of many crucial interactions in biological materials are often comparable to the thermal energy, as for instance in the case of hydrogen bonding, van der Waals interaction and static electronic interaction, etc. Biological materials show highly viscoelastic, since their response to mechanical load is intrinsically time-dependent. In many cases, biological materials contain extremely compliant structures, in which entropic contributions to free energy are important. Many interactions or forces which are not taken into account at macroscopic scales are no longer negligible, and should have significant effects on the measurements. Many material properties are size dependent and can vary significantly across various length scales. Quite often, the size effects are very strong and possibly utilized systematically to ensure physiological functioning of the material in its biological context. However, why and how these size effects are exploited within this context remains less understood.

V. PHONONIC CRYSTALS AND MANIPULATION OF ELASTIC WAVES

5.1. Phononic Crystal and its Unique Feature—Bandgaps

Since Kushwaha et al.[140] proposed the concept of 'phononic crystals' (PCs), marked success has been achieved in both theoretical and experimental studies for this kind of artificial acoustic functional materials. PCs, also termed 'acoustic bandgap materials', are composite media composed of periodic arrays of two or more materials with different mass densities and elastic properties. The constitutive materials may be either solid, liquid or air; the periodicity of the structures may be in one-, two- or three-dimension with the scatterers being layers, cylinders and particles respectively. The unique feature of PCs is that they may exhibit complete (or absolute) bandgaps in their transmission spectra where the propagation of acoustic or elastic waves is strictly forbidden in all directions (if not in all directions, then we have directional bandgaps). Two mechanisms can lead to complete acoustic bandgaps. One is the Bragg scattering in periodic systems. Symmetry, periodicity and order of the periodic system are all important to the existence of a 'Bragg-type gap'. To obtain a low-frequency gap, the size of the crystal must be large enough (even several meters in some cases). This limits the application of the PCs in low frequencies (say lower than 1 kHz). In addition, the requiring of the strict periodicity also brings the difficulty in manufacturing of the crystals. In 2000, Liu et al.[141] reported a new PC based on the localized resonance which is now regarded as another mechanism leading to bandgaps. They fabricated the crystal by arranging centimeter-sized lead balls, which were coated with 2.5 mm layers of silicone rubber, in an 8×8×8 simple cubic crystal with a lattice constant of 1.55 cm with epoxy as the hard matrix material. Two band gaps near frequencies of 400 Hz and 1350 Hz, which are two orders of the magnitude lower than the Bragg diffraction threshold, were observed by both experimental measurement and numerical calculation. This opens a way to application of PCs in low frequencies. The existence of a 'resonance-type gap' is determined by the resonance of the scattering unit and is independent of order, periodicity and symmetry unless there is a high concentration of resonating units so that they couple strongly with each other.

5.2. Characterization and Computation of Band Structures

Bandgaps for a particular PC are generally obtained by computing the band structures (i.e., dispersion curves) and transmission spectra, among which the transmission spectra are easily measured. Besides, the density of states and the localization length/factor[142, 143] are also used to characterize the bandgaps. The distribution of wave fields (e.g. displacement field, pressure field, etc.) can visually demonstrate the behaviors of wave propagation and localization under a particular frequency but is difficult to exhibit the spectrum properties.

The band structure or dispersion curve is no doubt the most important parameter to characterize the acoustic features of the PCs. Up to now, several methods have been developed to calculate the band structures. Except the transfer matrix (TM) method for one-dimensional (1D) systems, the existing methods may be divided into two main categories. The first one is the eigenfunction expansion methods (meshless methods), among which the plane-wave expansion (PWE) method[140] has been widely used. It expresses the displacement fields in the infinite sums of the plane waves (Fourier series). However it

converges very slowly for systems with a large acoustic mismatch or in three-dimensional (3D) case. It even fails to give accurate results for the mixed solid-fluid systems[144]. The recently developed wavelet method[145, 146] modifies the PWE method by replacing the Fourier basis with the wavelet basis. It improves the convergence rate and reduces the computational time significantly. The multiple scattering theory (MST) method[147] employs the cylindrical wave expansions and is only valid for circular or spherical scatterers.

The second category is the discretization methods (mesh or reduced-mesh methods), e.g. the finite element method (FEM), the boundary element method (BEM) and the lumped-mass method (LMM)[148], which discretize the unit cell (or its boundary) of a phononic crystal. All the above-mentioned three discretzation methods yield matrix eigenvalue problems from which the band structures can be calculated. Another widely used discretization method is the finite difference time domain (FDTD) method[149] which uses a different strategy. It calculates the time response of a unit cell and then obtains the eigenfrequencies using the inverse Fourier transform. Among all these methods, FEM and FDTD are the competitive methods because some standard commercial softwares, such as ABAQUS, COMSOL Multiphysics, etc. are available. However, the problems of convergence, stability, computational time and occupied memory of the computer may arise when a 3D system with defects is calculated. Some accelerated algorithms and/or parallel computing are necessary.

Most of the aforementioned methods, even PWE, Wavelet and MST methods when combined with TM, can be used to compute the transmission spectra. The density of states and the localization length/factor can be obtained from the band structures and the transmission spectra respectively, or can be computed by Green function method and TM method[143] respectively.

5.3. Manipulation of Elastic Waves and Applications

PCs are a competitive candidate to manipulate the elastic wave propagation because of its unique feature—bandgaps. The complete bandgaps could be engineered to provide a vibrationless environment for high-precision mechanical systems in given frequency ranges. Careful design of material combinations and structure parameters plays a crucial role for the appearance of a band gap. The location and width of the bandgaps concern mainly the mass density, elastic properties and volume fraction of the components as well as the topology of the structures (*incl.* the shape and size of the scatterers and lattice form). For instance, the large contrast of the material properties, especially the large density contrast of the components, is favorable for appearance of wider gaps[150]; the triangle lattice (for 2D case) and face-centered-cubic lattice (for 3D case) exhibit wider bandgaps[151]. Introducing random disorder[152] or quasi-periodicity[153] can also tune the bandgaps. Surface wave modes in a half-space system[145] and Lamb wave modes[154] in a PC plate may exhibit different band structures from bulk wave modes.

By breaking the periodicity of the systems, it is possible to create highly localized defect or guided modes within the bandgaps. This makes the PCs potential candidates for the design of elastic or acoustic microcavities, wave guides, filters, perfect mirrors, et al. For instance, removing a scatterer or replacing it by a different material will generate a point defect. The wave of particular frequency in the bandgap is localized at the defect. The point-defect state can be tuned by adjusting the material properties and geometry of the defect. This gives a way to design novel microcavities trapping the waves. A line defect, which is generated by removing or replacing a row of scatterers, will lead to the guided-wave modes propagating along the defect and even turn at a sharp 90°-corner without leak. This behavior is helpful in design of the highly efficient new waveguide. A plane defect with an array of scatterers in a plane removed or replaced acts as a perfect mirror for total reflection of waves[155]. A subtle design with combined line and point defects may produce an up-load/down-load filter, frequency demultiplier/divider, coupler or demultiplexer/splitter[156–158].

The existence of a bandgap may result in nonlinear distortion of the dispersion curves at the band edges, which will induce some surprising features of PCs, such as slow wave effect[159], negative refraction[160], negative elastic modulus or mass density[161, 162], collimation[163, 164]. Therefore the PCs show challenging applications in design of acoustic super lens[165], wave cloak[166], directional radiation[163, 164], etc. Gradient distribution of the scatterers' geometry, mass density or elastic moduli can modulate gradient variation of the effective refraction index, and thus control the wave propagation in PCs[167, 168]. This can also realize acoustic focusing, perfect reflection and wave guiding.

Other potential applications of PCs may include design of a mode-selecting acoustic filter by using resonant tunneling[169], sensor[170], energy harvester[171], thermoelectric device[172], etc.

5.4. Open Problems and Future Directions

(i) Improvement of the existing methods and development of the new effective and fast methods for band structure computation taking into account various interface conditions between scatterers and matrix and the attenuation of waves due to viscosity; development of accelerated and parallel numerical methods.

(ii) Application of new materials (e.g. piezoelectric/piezomagnetic materials[173, 174], ferroelectric materials[175], elastomer[176], etc) as components to modulate the bandgaps and realize the mechanical-thermo-electric-magnetic-optic multiple functions of PCs.

(iii) Homogeneous theory and equivalent continuum model of PCs, especially for high frequencies including strong dispersion.

(iv) Characterization and simulation of wave propagation in quasi-periodic PCs with applications; influences of disorder on wave propagation in PCs.

(v) Nonlinear wave propagation in PCs with or without defects.

(vi) Optimization of materials and structures of PCs to realize the desired acoustic functions[177].

(vii) Wave propagation in PC beams, plates and shells with or without defects and their applications in design of new acoustic devices.

(viii) Manufacturing of PCs, especially at micro- or nano-scale for very high frequencies (VHF)[178].

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