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Micro- and nano-mechanics in China: A brief review of recent progress and perspectives

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The past three decades have witnessed the explosion of nanoscience and technology, where notable research efforts have been made in synthesizing nanomaterials and controlling nanostructures of bulk materials. The uncovered mechanical behaviors of structures and materials with reduced sizes and dimensions pose open questions to the community of mechanicians, which expand the framework of continuum mechanics by advancing the theory, as well as modeling and experimental tools. Researchers in China have been actively involved into this exciting area, making remarkable contributions to the understanding of nanoscale mechanical processes, the development of multi-scale, multi-field modeling and experimental techniques to resolve the processing-microstructures-properties relationship of materials, and the interdisciplinary studies that broaden the subjects of mechanics. This article reviews selected progress made by this community, with the aim to clarify the key concepts, methods and applications of micro- and nano-mechanics, and to outline the perspectives in this fast-evolving field.

micro- and nano-mechanics, multi-scale and multi-field methods, nanotechnology, nanomaterials, nanostructures

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1 Introduction

Mechanics is a discipline with a long history, which studies the deformation and motion of physical objects in general, offering fundamental concepts, quantitative theories, computational methods and experimental tools for engineering applications. Micro- and nano-mechanics is a relatively new branch of mechanics that explores the mechanical behaviors of nanostructures and the micro-/nanostructure-properties relationship of bulk materials with fundamental mechanical processes occurring at the submicron length scales [1,2]. The field nucleates from the continuous size reduction in the microelectromechanical systems (MEMS), the vast discovery of nanomaterials and nanostructures, and the fast development of nanotechnology in a multi-disciplinary context [3]. It uncovers new physics in the material deformation, fracture and flow at the nanoscale that are distinct compared to the behaviors of a conventional continuum, and offers theoretical insights, computational and experimental tools for the ongoing exploration [3,4].

Along with the continuous down-sizing in the semiconductor industry, materials have been fabricated in forms of quantum dots, nanowires and thin-films. The size reduction into submicron scales endows prominent quantum confinement for the electrons, and raises the significance of surfaces and interfaces in their mechanical responses. The discovery of nano-carbon with sp^2-hybridized covalent bonding networks such as the fullerenes, carbon nanotubes

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(CNTs) and graphene with the single-atom thickness pushes further the limit to the extreme low-dimensional regime (Figure 1). The concepts, assumptions and validity of continuum mechanics are challenged by a wide spectrum of problems raised at this scale as the consequence. For example, the mass and energy densities cannot be well defined due to the failure of continuity assumption; thermal fluctuation inevitably modulates the mechanical behaviors of nanostructures; the material nonlinearity and anisotropy could develop from the discrete lattice symmetry and low dimensionality. Exploration has been urged to address these issues, which not only brought in new ideas that widen the conventional understandings, but also offered chances to revisit the paradigm developed in the past.

Appearing as a surprise at first but later widely accepted, the continuum models of shells and beams can be applied to assess the elastic response and even mechanical stability of single-walled CNTs (SWNTs) [5] and multi-walled CNTs (MWNTs) [6] that are narrow tubules with diameters down to a few nanometers. Studies have been inspired by these exciting discoveries, and a multi-scale theoretical framework rises to the surface by coupling the scale-free stress and strain fields in continuum mechanics to the underlying lattice dynamics. Within this framework, the understandings acquired at the nanoscale iteratively help to improve theories in the continuum mechanics with physical consideration of the microscopic mechanisms. Microstructural characterization techniques were developed with the atom-level resolution under electron microscopies [7,8], optical spectroscopy [9], as well as X-ray synchrotron and neutron scattering techniques. Equipped with *in-situ* mechanical apparatus, deformation and failure processes could be directly visualized, which elucidates microscopic origins of the mechanical performance of bulk materials, and reveals the unconventional behaviors of nanostructures and their assemblies (Figure 1). The research conducted in these directions incubates innovative mechanical designs, for instance, to achieve the strengthening-toughening synergy, structural super-lubricity, super-hydrophobicity and highly-slippery fluid flow.

At the submicron scale, mechanical behaviors of materials can be coupled to other fields with the ease of creating significant strain, size and surface (interface) effects. A multidisciplinary approach would thus help to bring deformation and motion into the development of functional materials and devices as the additional dimensions of performance control. For instance, defect-, strain-, surface (interface) engineering, and applying external cues such as forces or fields have emerged as general strategies in material and device design [10,11]. Studies on the interfaces between nanomaterials and living systems also deliver fruitful understandings of biological systems and stimulate technological development in biomedical engineering. These advances clearly demonstrate the role of mechanics as a driving force of innovation in the technology frontier.

In the 1950s, Tsien [12] brought up the idea of physical mechanics as a "new engineering science" to "predict the engineering behavior of matter in bulk form from the microscopic properties of its molecular and atomic constituents". The proposal is called upon to address the need from jet propulsion, aeronautics and atomic power, and its impact is "inevitable on all fields of engineering". After half-century development in the computational facilities and tools for large-scale atomistic simulations and experimental techniques that are able to probe material behaviors across multiple length and time scales from the atomic level, the barrier to solve problems with microstructural complexity is reduced, and a scientific paradigm shift in mechanics may emerge. The science of micro- and nano-mechanics has many facets, which have been well documented in recently published monographs and textbooks that summarize the exciting achievements [3,4,13]. It is impossible to review all

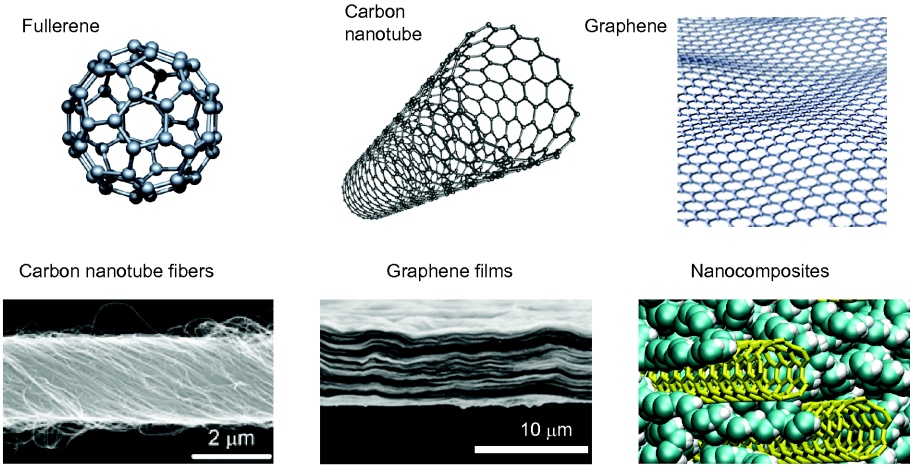

Figure 1 (Color online) Representative low-dimensional carbon nanostructures, their interfaces and macroscopic assemblies in forms of fibers, films and nano-composites.

of the advances made by the Chinese community in this single article, and instead we choose to offer a few vignettes of the vast endeavor with focus on several major concerns. The presentation is limited by the knowledge of the authors, nonetheless, we hope that the summary and perspectives serve well to illustrate how the research contributes to the discipline of mechanics, and the development of nanotechnology.

2 Mechanics at micro- and nano-scale

2.1 Mechanics at low dimensions

2.1.1 The very thin nature

CNTs and graphene feature outstanding mechanical properties. Moreover, their mono- or few-layer nature allows structural tailoring at nanoscale, as well as physical and chemical modifications that are accessible to every atom in the materials, in principle [10]. Many of these merits are shared by other low-dimensional materials such as silicon nanowires and 2D transition metal dichalcogenides. A wide spectrum of applications ranging from the space elevator, the optoelectronic devices to structural and functional nanocomposites have been proposed and investigated. As structural components, these low-dimensional nanomaterials can be single-atom-thick, and thus the mass and energy density distributions are delta functions in space. Consequently, a thickness has to be defined to formulate a continuum theory. One may use the interlayer distance of graphite, 0.335 nm, as the nominal thickness of sp^2 carbon nanostructures, with which one has the Young's modulus and tensile strength of graphene sheets as $Y = 1$ TPa and $\sigma_S = 120$ GPa. However, it should be noted that the bending resistance of low-dimensional crystals such as graphene originate from the interaction between π-orbitals of neighboring atoms in the lattice, which is different from the sp^2 or σ orbitals that contribute to the in-plane mechanical resistance. The result from this link of mechanical properties to the chemistry is distinct. If the bending response is involved in the plate or shell model of low-dimensional materials, the so-called "thin-shell thickness" has to be defined to conform to the relation between the Young's modulus and bending stiffness, which is one order lower than the nominal thickness [14,15]. It should be further noted that the thin-shell model of sp^2 carbon nanostructures becomes size-dependent at high curvature due to the rising of sp^3 hybridization in the covalent bonding network [16,17]. The contrast in the high Young's modulus and low bending rigidity ($\kappa = \sim 1$ eV) of a 10 μm×10 μm graphene sheet leads to highly anisotropic mechanical responses with a Föppl-von-Kármán number, $\mathrm{FvK} = YL^2/\kappa$, that is comparable with that of an A4 paper. The direct evidences of this anisotropy include the formation of ripples and wrinkles [18-23], which are highly nonlinear phenomena resulted from the mechanical instability [24].

Fundamental parameters characterizing the deformation of sp^2 carbon nanostructures including the fullerenes, CNTs and graphene were calculated from atomistic simulations by fitting to the continuum models [25]. These parameters include the bending stiffness in response to the change in mean and Gaussian curvatures, where the latter is obtained from calculations of fullerenes with the lattice topology measured by the number of pentagons or heptagons, in addition to that of the hexagons. The *Theorema Egregium* of Gauss says that the Gaussian curvature is a bending invariant upon isometric deformation in the absence of in-plane stretch [26]. As a result, the Gaussian bending stiffness creates a connection between the in-plane and out-of-plane elastic responses with changes made in the lattice topology. A nonlinear continuum theory could thus be formulated for the low-dimensional structures, with the ability to include the lattice topology in mechanical design [27,28].

2.1.2 Lattice discreteness and symmetry

With the length scale reduced down to a few nanometers, the effects of lattice symmetry and discreteness become pronounced. The mechanical stability of low-dimensional structures was discussed based on an energy-based criterion, concluding that 1D monatomic chains, 2D honeycomb lattices, square lattices, and triangular lattices are the only four permissible structures [29]. The propagation of flexural wave with short wave lengths and the growth of buckling-driven wrinkles in graphene demonstrates a six-fold symmetry, which contradicts with the isotropy of 2D elasticity as concluded from the hexagonal lattice symmetry, can be attributed to the development of lattice distortion at finite strain [19,30]. Negative Poisson's ratios were predicted for the single-layer black phosphorus and graphene nanoribbons, which originate from the puckered lattice structure or the warped geometry [31,32]. More astonishingly, it was found that significant exotic lateral strains can be introduced while bending 2D crystals such as transition metal chalcogenides, resulting in a finite bending Poisson ratio—the ratio between the lateral strain and the curvature of bending, which is absent in the conventional theory of elasticity [33].

2.1.3 Defects

As a local mechanical perturbation in forms of stress or strain decays as r^{-D} at a distance r from its source, the significance of defects in a low-dimensional lattice with $D = 1$ or 2 is expected to be more prominent than that in 3D lattices [34]. The 2D forms of sp^2 carbon such as graphene then offers an excellent model material to explore the mechanical behaviors of defects, which can further be controlled in experiments [35] (Figure 2). It should be remarked that the theory of topological defects such as dislocations and disclinations were formulated in 2D, which could be used to analyze the stress and strain fields by neglect the out-of-plane distortion

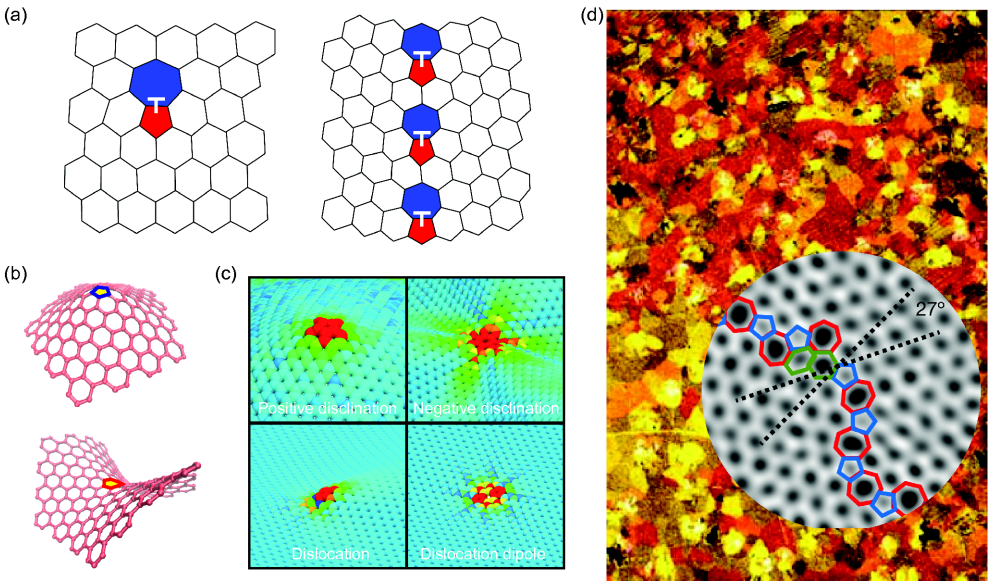

Figure 2 (Color online) Defects in 2D crystals. (a) Dislocations and grain boundaries in a hexagonal lattice. (b) Warping of 2D crystals with a single positive (top) and negative (bottom) disclinations. (c) Out-of-plane distortion of 2D crystals with typical defects. The color depicts the bonding energy of atoms. (d) Polycrystalline texture of graphene films. The arrangement of dislocations in the grain boundaries, i.e., the pentagon-heptagon pairs, are shown in the inset [36].

that releases elastic distortion near the defects [37,38]. The theory then allows the prediction of polycrystal strength following the experimental evidence that the topological defects (TDs) composed by pentagon-heptagon (5-7) pairs constitute the grain boundaries (GBs) [37,39]. In a bi-crystal, the GB strength is determined by the density of TDs and their arrangements. The strength of a tilt GB increases as the square of the tilt angle if the 5-7 pairs are evenly spaced, and the trend breaks down in other cases [37]. In the polycrystal with tri-GB junctions, a pseudo Hall-Petch size dependence of the strength was uncovered, which decreases with the grain size a as a result of the stress accumulation (~log$a$) along the straight GBs consisting of oriented 5-7 pairs [39]. To reduce the accumulation of lattice distortion and stress buildup, long, straight GBs prefer to split into short segments during the growth process, while the latter result in local stress buildup in the polycrystalline texture only. The consequently statistical size dependence of strength that increases with the grain size can be understood through the weakest-link theory, which could also account for other types of defects that create local stress buildup [34,40].

In-situ mechanical tests under the scanning electron microscopy (SEM) have been carried out to assess the mechanical performance of low-dimensional materials, which unsealed the theoretical limits of elastic strain (~16%) and strength (~20 GPa) of single-crystal silicon nanowires with very low concentration of defects [41]. The in-plane mechanical properties of MoS_2 were also investigated by *in situ* tensile testing, demonstrating a transition from inter-planar failure for thick films to intra-planar fractures for mono- or few-layer sheets [42]. Directly measuring the tensile strength of defect-free graphene is technically challenging, as the weak van der Waals interface between graphene and other materials in contact usually cannot provide sufficient clamping forces. Instead, notched samples were prepared that allow fracture toughness to be measured [43]. Nanoindentation tests have been used alternatively to measure the elastic response and fracture strength of 2D materials, which report consistent values with the theoretical predictions [44,45]. However, it is shown that this local probe of material strength is sensitive to the local lattice topology and the out-of-plane distortion, which cannot be directly mapped into the in-plane mechanical resistance of materials through a simplified model of a flat membrane [46]. As a demonstration of the geometrical effect, the apparent stiffness of graphene under nanoindentation was found to surprisingly increase vacancies at low concentration, which is explained by the combined effect from defect-induced swelling of the graphene sheet that stiffens the mechanical response due to the distorted geometry, and softening of the in-plane lattice upon defect creation [47].

2.1.4 *Fracture*

The fracture pathway in brittle 2D materials is determined by both the loading condition and the anisotropy in the cleavage energy density [48]. The edge energies of 2D crystals are orientation-dependent due to the lattice symmetry, which leads to the difference in the packing density of atoms in the lattice planes or lines. It was shown that the Griffith criterion formulated through the cleavage energy density fails to

capture the dependence of fracture strength on the crack length for nanoscale short cracks, and a force-based criterion following the Inglis formulism should be used instead [49]. The out-of-plane distortion of lattice near the cracks could increase the elastic energy release rate and thus reduces the Griffith strength [50]. Moreover, one should note that unlike most brittle materials that break below a strain of ~5%, the perfect lattice of low-dimensional crystals such as graphene and CNTs could bear remarkably large elastic strain up to 20% [44]. The nonlinearity and changes in the edge cleavage energies at high strain levels may further revise the linearly elastic fracture mechanics based predictions.

2.1.5 Anisotropy in multilayers

The mechanical responses of MWNTs, CNT bundles and graphene multilayers (including graphite) are highly anisotropy because of the weak van der Waals interaction between the graphene layers [6,51]. By defining a degree of anisotropy $\delta = \frac{\|\mathbf{C}-\mathbf{C}_{\text{iso}}\|}{\|\mathbf{C}\|}$ for the elastic stiffness tensor $\mathbf{C}$, where $\|\cdot\|$ is the standard norm and $\mathbf{C}_{\text{iso}}$ is the isotropic component, it was found that graphite possesses the highest anisotropy degree as well as the lowest ratio between shear and Young's moduli, compared to all other known hexagonal crystals. The SWNT bundles features even higher degree of anisotropy and lower modulus ratio than those of graphite [52]. This extreme anisotropy in the stiffness and strength limits the load transfer between nanostructures and their environment [53], leading to the frequently-observed failure mode through interfacial sliding [54,55], as well as the anomalous vibrational and buckling behaviors of the multilayers [51,56,57]. A continuum mechanics based model is practically useful to assess the load bearing capability of the nanotube bundles or layered assemblies, as well as and their nano-composites, which, however, can only be formulated with an energy density defined for the interlayer space that features a larger length scale than the in-plane lattice constants. Following the spirit of shear-lag-type models [58], one could include the interfacial space where the mechanical coupling is manifested into a representative volume element (RVE) that is defined to explore load bearing in the nanostructures and load transfer across their interfaces [59,60]. However, the lack of mass assigned to the interlayer phase need to be further clarified, especially when the dynamical effects are concerned.

2.2 Micro- and nano-mechanics for nanostructured bulk materials

The study on the mechanical properties of metals and alloys presents an excellent example of success in applying the top-down multiscale mechanics approach (Figure 3). The phenomenological theory of macroscopic plasticity for metals and alloys has been revolutionarily revised since the introduction of microscopic concepts such as dislocations, twins and phase transformation into the continuum framework [61]. Macroscopic samples of metals and alloys are highly complex in their chemical composition, textures and microstructural defects [62], the mechanical properties of which may feature explicit dependence on time, stress/strain and temperature [63,64]. With the evolutional rules clarified for dislocations, grain boundaries, displacive transformations (martensitic transformation, twinning), microstructure-informed crystal-plasticity or phenomenological theories can be constructed, improved by electron microscope and molecular simulation based studies, and then used for large-scale applications [61,65-67]. This mapping from atomic-level mechanisms into the continuum formulation of material deformation and failure successfully balances the complexity in microstructural information and abstraction in theory [61], to give "a satisfactory representation of reality" [12]. This is of critically importance to develop engineering applications, where the materials are manufactured by stable processing procedures, and the mechanical performance of materials are characterized by a set of parameters not varying with microstructures.

The multiscale understandings could advise the development of bulk materials with elevated mechanical performance, which could potentially resolve the strength-ductility trade-off resulted from the monotony in the microscopic

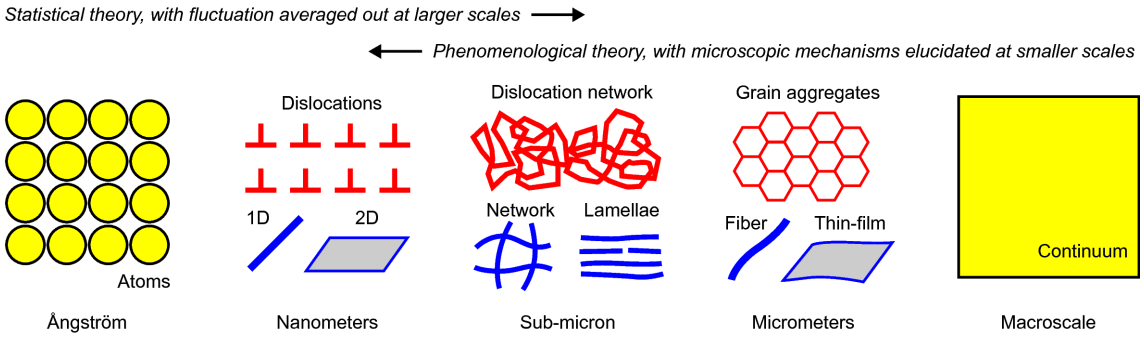

Figure 3 (Color online) Multiscale representations for the mechanical performance of metals (top) and nanostructured macroscopic assemblies in forms of fibers and films (bottom).

mechanisms of material deformation. One central idea is to separate the strengthening and toughening mechanisms at different length scales or hierarchical levels, which has been addressed in a number of studies combining microstructural characterization under SEM, and the transmission electron microscopy (TEM), as well as computer simulations from the atomistic, dislocation to the continuum level [68-83]. Dislocation strengthening of metastable austenitic steels without ductility trade-off was achieved by decoupling the two mechanisms—the yield strength is controlled by initial dislocation density while ductility is retained by the capability to nucleate new dislocations that accommodate plastic deformation [84]. Heterogeneous structures with soft lamellae micro-gains embedded in the hard ultrafine-grained lamella matrix offer unusually high strength with high back stress developed from the heterogeneous yielding, and high ductility resulted from back-stress and dislocation hardening [85]. A dual-phase design of nanostructuring combining the benefits from nanocrystallinity and amorphization was proposed, which yields the strongest magnesium-alloy consisting of nanocrystalline cores embedded in glassy shells, where the crystalline phase blocks the propagation of localized shear bands under straining, and within any shear bands that do appear, embedded nano-grains divide and rotate, contributing to hardening and countering the softening effect of the shear band [86]. The grain-level gradient structure induces a macroscopic strain gradient upon loading, which promotes the accumulation and interaction of dislocations, resulting in extra strain hardening [87], and enhances the fatigue resistance of steels [88]. Gradient nano-twin structure could also evade the strength-ductility trade-off, doubling the strength of steel at no reduction in ductility [7]. The recent activities in bulk metallic glasses [89-95] and high-entropy alloys [96] added new dimensions to the design space of bulk materials with engineered atomic-scale spatial and compositional orders.

Compared to the micro- and nanostructuring engineering in bulk metals and alloys, the bottom-up fabrication of nanostructure-based materials takes the advantage in the structural tailoring and surface (interface) modifications (Figures 1 and 3). The structural hierarchy in macroscopic assemblies of nanostructures, in forms of fibers, films, foams and nano-composites is reminiscent of biological materials such as nacre, bones and silks [97-100]. In contrast to the metals with commonly closely-packed lattices, the porosity and hierarchy of these materials introduce microstructural complexity that cannot be explicitly formulated within a continuum framework. The evolution of microstructures under loading and load transfer through their interfaces are the two key processes defining macroscopic mechanical behaviors [59,101-106]. For example, recent studies revealed the microstructural evolution of CNT fibers under tension, where elasticity, strengthening and damage-failure in the mechanical responses were discussed based on a two-level interfacial model that captures the bundling nature of fibers [9,55,107], and it is shown that the strengthening-toughening synergy can be implemented by introducing multimodal interfacial interactions or structural hierarchies into the assemblies of nanostructures [102,108-111]. However, current exploration has mostly been limited to closely-packed nanotube bundles [112] and layered assemblies [112], where the RVE approach is feasible. Abstraction of the complex microstructures and their evolution under mechanical loading has, however, not yet been achieved. As alternative routes for bottom-up fabrication where the microstructural complexity can be controlled by design, the recent advances in additive manufacturing, namely 3D or 4D printing, and guided assembly of rationally optimized microstructures enable the development of architectured and morphable materials [113-117].

2.3 Micro- and nano-mechanics at surfaces and interfaces

2.3.1 Surface and interface effects

With the reduction in dimension, surface and interface effects become important in defining the mechanical responses of structures [118,119]. By defining an individual phase of surface layers or the interface/interphases, the deformation and vibration of microstructures can be theoretically modelled in the framework of continuum mechanics [119]. In the spirit of the Gurtin-Murdoch theory [120-122], the surface is assumed to be a zero-thickness elastic layer attached to the bulk, where the surface energy density and stress follow a linearly-elastic constitutive relation, and a set of surface elastic constants are then introduced to characterize the surface properties. The theory was recently revisited from an orbital-free density functional theory (OFDFT) perspective, based on which the explicit expressions of surface elasticity parameters can be derived [123]. The surface effect under an applied electric field was also discussed with the consideration of surface charge distribution [124]. A surface (interface) theory was then developed for finite-deformation elasticity, where the curvature-dependence of interface energy and residual elastic fields were considered [125-127]. Recently, an alternative surface energy density based elastic theory was developed, where the surface-induced traction related to the surface stress was identified as a function of the surface energy density. The surface relaxation parameter and surface energy density of the bulk material serve as two material parameters instead of the surface elastic constants [128]. The study was extended for the interface effect, where the interface energy density is considered as a function of bulk surface energy densities, while the surface relaxation and mismatch parameters of the two phases constituting the interface instead of the interface elastic constants [129].

These efforts clarified the size-dependent elastic behaviors of nanostructures such as nanoparticles, nanowires and nanosheets, and the overall properties of nanocomposites with surfaces or interfaces embedded [130-143]. With further size reduction, the mechanical behaviors of surfaces and interfaces in atomistically thin materials become even more intriguing.

2.3.2 *Solid interfaces*

The study on interfaces between micro- or nanostructures was initialized by technical challenges in the MEMS technologies, where the strong adhesion, friction and wear are major problems limiting both the yield of fabrication and the lifetime of operation in MEMS devices. For example, the adhesion or stiction can be a fundamental issue concerning the reliability of MEMS, which has been studied using the microscale elastic and elastoplastic adhesion-contact theories. Dimensionless parameters such as the Tabor number, the peel number, the adhesion parameter for the elastic adhesion-contact, the plasticity index of for the elastoplastic model were defined, and models were constructed to characterize the key mechanical processes [144].

Friction between solid surfaces is intrinsically an atomic-scale process, which, however, is averaged out in macroscopic phenomena. Consequently, at a length scale that is much larger than the one corresponding to the microstructural irregularity, roughness or the localized deformation of surfaces, empirical rules such as the Amonton's law apply. 2D materials such as graphene with atomistically smooth surfaces demonstrate different behaviors. By cleaving graphite blocks, a six-fold symmetry of interlayer lattice registry is identified, which clearly demonstrate the discrete lattice symmetry arising from the interfacial commensurability [145]. The ultralow friction between incommensurate graphite surfaces permits fast retraction motion as a result of the interfacial tension [146], which can be analyzed to measure the cleavage energy [147]. The values of friction force or energy barriers against the translation motion in this structural super-lubric regime can be extracted from the distinct temperature dependence of retraction dynamics [148]. As the thickness of graphite shrinks down to single- or few-layers, the development of contact quality in consequence of the structural flexibility of thin sheets leads to prominent layer-number-dependent frictional characteristics on an adhesive surface [149]. Coupling between the elastic deformation of graphitic layers and their interlayer shear or sliding should then be accounted for, to bridge the microscopic lattice dynamics to the mechanical responses of macroscopic samples. In addition, the mechanical energy dissipation, manifested through the vibrational mode coupling, defines the lifetime of devices that operate in the structural super-lubric regime [150-152], which remains as an open question due to the lack of a theory for the nonlinear dynamics of lattices.

The interfaces between low-dimensional nanostructures and matrices are critical for the load and energy transfer in nano-composites. Theoretical models based on the shear-lag theory and fracture mechanics are developed to predict the criterion and process of interfacial failure [108,153], and *in-situ* experiments were also designed to measure the interfacial shear resistance between 2D crystals, as well as their interfaces with the polymer matrix, where micro-Raman spectroscopy was applied to map the strain field in carbon nanostructures interfaced with others or the matrices, concluding that these interfaces are usually the weak points to fail under loading [9,55,154-156]. These studies lay the ground for the interface engineering of the assemblies of nanostructures and their nano-composites with elevated mechanical performance. In practice, the interfaces can be modified through interlayer crosslinks [157] that improve the mechanical performance of the layered assemblies of 2D materials [59,158], offering strong, tough and self-healable fibers or films if multimodal crosslinks are introduced [108]. The strong-weak duality in the in-plane mechanical resistance and out-of-plane flexibility of graphene also allows one to design shock-resistant layered nano-composites, where the low bending stiffness leads to interlayer reflection that weakens the shock wave, while the strong in-plane sp^2-bonded lattices constrains dislocations and heal the material [159].

2.3.3 *Solid-liquid interfaces*

Wetting is a common and compelling phenomenon, with research driven by both curiosity and industrial needs. Micro- and nanostructures have been widely applied in the design of functional surfaces with super-hydrophobicity, for example. Partial wetting of a surface with air trapped in microstructures, termed as the Cassie-Baxter regime, plays the key role in increases the water contact angle [160], while mechanical perturbation or gas diffusion could drive the transition into the fully-wetted Wenzel mode [161,162]. The microstructural parameters can be modified for preferred surface wetting properties. A Cassie-Baxter mono-stable super-repellent materials can be fabricated [163], and the ultimate stable underwater superhydrophobic state can be achieved by the synergy of mechanical balance and chemical diffusion equilibrium across the entrapped liquid-air interfaces [164]. The wetting dynamics on the superhydrophilic surfaces can be engineered by the texture of microstructured surfaces [165]. Directional motion of droplets can be driven by the surface curvature [163] and the topological design of the microstructural patterns of the substrate [166]. The effects of microstructural features on the sliding behaviors and friction of droplets on hydrophobic surfaces were also explored [167,168]. For the motion and phase change of liquid droplets on a solid surface, where the movement of triple-

phase contact lines is involved, a multiscale approach is required to resolve the so-called Huh-Scriven paradox. Specifically, the presence of precursor films ahead of the nominal moving contact line is proved to be the first answer to the stress singularity and infinite energy dissipation in electro-wetting [169-171]. A multiscale method including both the viscous resistance at mesoscale and the molecular friction at microscale in the triple-phase region was developed to explore the dynamic wetting of a droplet on a pillar-arrayed surface [165,172].

The atomistically smooth, non-polar and chemically inert graphene surface demonstrates ultralow friction for liquid flow that features a layered order near the surface [173]. The interfacial mechanical resistance can be quantified by the critical shear stress, and the energy dissipation could be evaluated from the potential energy landscape following the molecular kinetics theory [135]. The significant boundary slippage predicted for liquid flow confined in nanochannels such as the CNTs and the interlayer gallery between graphene sheets was validated by directly measuring the rate of water flow through individual ultralong CNTs and graphene channels [174,175]. It was further shown by molecular-kinetics-based analysis that the liquid slippage on a solid surface is correlated to the interfacial adhesion [176]. More interestingly, the lattice strain and vibration of the nanochannel walls could significantly modulate the fluidic transport [177,178]. Such a mechanism is expected to enable fast permeation of water through graphene-derived membranes, where graphene channel networks could form an efficient transport pathway [179,180]. However, it should be noted that the oxygen-containing surface functional groups in the graphene oxide sheets could break down the flow enhancement endowed by the remarkable interfacial slippage [173], and the complete understanding of convective or diffusive mass transport processes can only be reached by elucidating the transport pathway embedded in the lamellar membranes of 2D materials [181]. Strikingly, the solid-liquid interface allows hydroelectric voltage generation, for example, through the interaction between the moving chain of water dipoles and the charge carriers in CNTs [182], or nanostructured carbon materials [183]. Moving the liquid-gas boundary along a graphene sheet could also induce drawing and waving potentials [184,185]. The drawing potential arises due to the simultaneous charging and discharging of pseudo-capacitors in front and at the rear of the droplet, while the generation of waving potential is attributed to the charge transfer driven by the non-equilibrium electrical double layer (EDL) near the liquid surface. The coupling between molecular dynamics and electronic excitation extends the family of electro-kinetic phenomena and offers a brand new concept of design for energy conversion applications [184,185].

2.4 Model and method developments

2.4.1 Structural models

Low-dimensional nanostructures can be naturally modelled into beams or shells for quantitative mechanical analysis [6,16,186]. Based on these models, bending motion of CNTs driven by force or thermal fluctuation has often been used to measure the elastic response of nanostructures. It was shown that while considering the CNT as a continuum beam, the Euler-Bernoulli approximation fails by overlooking the shear effect under flexural deformation with a short wavelength. As a result, Timoshenko model with non-local elasticity should be used to account for the shear effect and rotational inertia [187]. Moreover, quantum statistical effects become prominent for the fluctuating motion at temperature significantly lower than the Debye temperature [188]. The anisotropy between strong covalent bonding in nanostructures and weak non-bonding interfaces between them could break down the deformation affinity in the assemblies of nanostructures such as the graphene multilayers. The impact is subtle in the fact that both the Euler-Bernoulli and Timoshenko models cannot capture the bending deformation of graphene multilayers, where significant interlayer sliding is characterized [56].

To model the single-atom-thick layers of CNTs or graphene in the elastic shell theory, a lattice-to-field correspondence has to be made, where the displacement of atoms can be mapped to the continuous displacement and strain fields, and thus used for the calculation of stress field through the interatomic interaction potentials [189]. The original and high-order Cauchy-Born rules play a central role in the implementation of constitutive models for the materials in the atomic representation by establishing mapping between the deformation field and atomic displacements, which were successfully applied to nanostructures such as CNTs and graphene [16,190-194]. Computational methods such as the atomic-scale finite element method (AFEM) were also developed to provide a seamless multiscale framework for large-scale elastostatic problems [195,196].

2.4.2 Multiscale methods

To understand how a material fail is the holy grail of solid mechanics studies. However, the nucleation and propagation of cracks in materials is an intrinsic multi-scale problem. Although the middle- and far-field behaviors of the cracks can be solved thanks to the early development of fracture mechanics, the crack tip is discontinuous and atomistic treatment has to be taken. In the framework of continuum mechanics, there are singularities in the stress, strain and displacement fields at the crack fronts, which cannot be resolved without the knowledge of detailed atomic structures. A multiscale, or trans-scale approach has then to be taken [197]. Since the 1980s, the advances in computational

hardware and software allow one to model the materials as an assembly of atoms, through their interactions modelled by empirical functions of the atomic structures, or electronic structures based calculations. To solve this problem, a three-scale framework was proposed by combining the atomic description for the crack front, the superelastic/viscoplastic models for the macroscopic deformation and the dislocation dynamics models for the intermediate mesoscale region, where two "hand-shaking" bridging zones communicate the information of stress and strain [198,199].

In a broader context, mechanics of materials mainly concerns the behaviors of structures at the length and time scales that are relevant for their applications (Figure 3). However, all of them have their origins from the atoms and their interatomic interactions. Many phenomena, such as material deformation, damage and fracture, are essential atomistic processes, where atomic bonds are distorted or broken under mechanical loads that are transmitted across multiple time and length scales. Consequently, linking material behaviors at different length and time scales is of extreme importance for material and structural design, where rational reasoning based on experimental evidences and statistical averaging approach are both essential [200]. Although general frameworks of multiscale theory and algorithms have been constructed [70-72,198,199,201-214], the computational cost would still be high if both the atomic-scale spatial resolution acquired for the physics and the large length scale concerned for the applications are both acquired. Phenomenological models would resolve this issue if variables can be introduced to characterize the microscale deformation and fracture mechanisms, as well as the rules of their evolution (Figure 4) [61,111,215-217].

3 Inter-disciplinary studies at micro- and nano-scale

3.1 Nano-devices and multi-field coupling

The unique properties of nanostructures have driven the proposal and development of novel opto-electro-mechanical devices. Gigahertz mechanical MWNT oscillators were proposed based on the inter-shell motion, which is driven by the surface tension between concentric graphitic layers [218]. The friction between atomistically smooth surfaces in the MWNTs is ultralow, and even thermal fluctuation can induce mechanical motion with amplitude significantly larger than the lattice constants [219]. Directional motion of CNTs can be powered by a temperature gradient due to the thermophoretic force originating from changes in the inter-wall van der Waals cohesion and an unbalanced edge force [220,221]. The intra-shell cohesion in CNTs with large diameters can induce successive collapse through a Domino wave with a speed up to 1 km/s [222], and the process can be reversed by heating up the bi-stable system [223]. Wrinkles formed at graphene interfaces can also be driven as soliton waves by thermophoresis, which could enable the so-called wrinkle engineering as their electronic structures are sensitive to mechanical deformation [23,224].

The coupling between mechanical deformation and other physical fields is remarkable at nanoscale, due to the feasibility to achieve a high level of local strain and strain gradient as well as the field strength [11,225]. For example, exceptionally large axial electro-strictive deformation (10% strain for field strength of 1 V/Å) can be induced in SWNTs by the electrical field, with volumetric and gravimetric work capacities three and six orders higher than those of best-known ferroelectric, electro-strictive, magneto-strictive materials and elastomers [226]. On the other hand, strain and strain-gradient engineering has been widely applied to modulate the properties of functional materials and physical processes therein. Piezoelectricity and flexoelectricity are two well-known examples demonstrating the feasibility. Theories were developed for these electromechanical phenomena, showing that for nanostructures, the size and surface effects result in strong coupling between the electric polarization, electronic structures, magnetism and strain or strain gradient [227-236]. Recent studies also conclude that reversing the applied stress can change the tunneling barrier sufficiently to produce a giant electro-resistance effect in the ferroelectric tunneling junctions [237,238]. The strain effect is also demonstrated by inducing and controlling the evolution of vortex domain patterns in ferroelectric nanostructures [239,240], or modulating thermal and electrical transport processes in the molecular junctions [241,242]. Beyond the

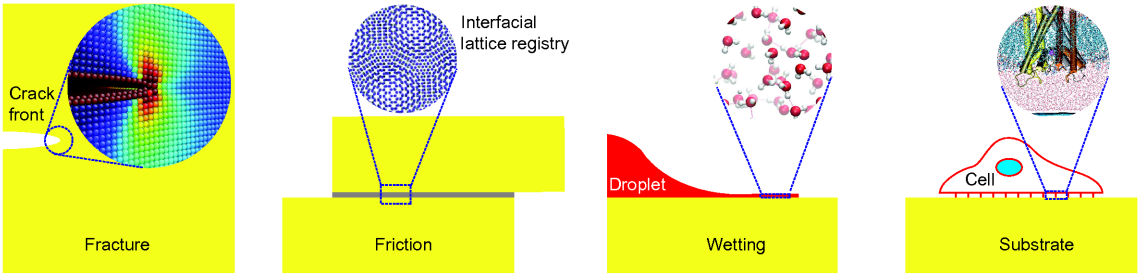

Figure 4 (Color online) Examples of multiscale problems where micro- and nano-mechanics are concerned-fracture, friction, wetting and behaviors of bio-interfaces.

electromechanical effects, the interplay between mechanical, optical, thermal and chemical processes at nanoscale has also driven notable research interests in developing models with fully coupled governing equations, boundary and interface conditions for the chemomechanical and mechanochemical processes such as creeping, oxidation and lithiation, as well as the photo-/pH-sensitive responses of polymers [243-250].

3.2 Mechanics at the bio-nano-interface

The interface between living matters and micro/nanostructures plays a crucial role in biological and biomedical processes such as biomedical diagnostics, therapeutics, and nanotoxicity, which has received an enormous surge in research interest. Cells actively sense the mechanical behaviors of the extracellular matrix [251], and cell-induced traction forces at the cell-matrix interface influence the processes of cell signaling, migration and tissue morphogenesis, among others [252]. Mechanobiological mechanisms that regulate the cellular processes have been elucidated by exploring the mechanical effects on cellular behaviors as a multiscale problem [253-255]. The cellular uptake process of nanoparticles was shown to be very sensitive to the geometry, rigidity of nanoparticles and the interfacial adhesion [256-259]. Theoretical analysis and molecular simulations show that the aspect ratio of nanoparticles and their adhesive interactions with the host medium plays key roles in establishing anomalous diffusive behaviors, with significantly higher diffusivity than their spherical counterparts in biological porous media such as mucus and tumor interstitial matrix [258,260]. These quantitative studies clearly demonstrate the importance of mechanical processes in modulating the behaviors of living system, the understanding of which could provide guidelines for a wide range of biomedical applications. However, it should be noted that because of the low characteristic energy scale associated with molecular interaction at bio-interfaces, the stochastic nature of molecular binding/unbinding events activated by thermal excitation could influence the interaction and kinetics, which should be carefully tackled [261].

4 Outlook

This brief review has been prepared based on recent progress achieved in the Chinese community of micro- and nanomechanics, which advances the theory and methods beyond those in the conventional continuum mechanics framework, and promotes innovative, interdisciplinary studies as demanded from the fast-evolving technical development and engineering applications in the new era of nanoscience and technology. In this final section, we highlight some of the unsolved issues in this field to stimulate further discussion and investigations.

There are still puzzles remaining with respect to the fundamental mechanical properties of nanostructures. The measured bending stiffness of the single-atom-thick graphene sheet is reported to be 4 orders higher than theoretical predictions, and thermal ripples induced renormalization was proposed, trying to fill the gap [262]. However, the interaction between mechanical deformation and thermal fluctuation still lacks clarification. The dislocation and disclination theories with the consideration of out-of-plane distortion have not yet been formulated for the TDs. The discussion of fracture processes even in the simple hexagonal lattice of graphene is not conclusive, not to mention that in curved nanostructures such as the 1D tubular or 2D warped. Rigorous models have to be developed for the study of low-dimension structures, by incorporating their lattice symmetry, geometrical distortion that could be highly nonlinear, as well as the explicit effects of thermal fluctuations. New tools to manipulate and probe mechanical deformation and motion at nanoscale should also be devised to validate the theoretical models [263-265].

Secondly, theories and computational methods are urged to predict the mechanical behaviors of materials with complex, evolving microstructures and their development during fabrication processes. Key indicators for these features have to be identified, and preferably, implanted into continuum models as microstructure-sensitive variables to balance the abstraction and feasibility acquired in engineering applications. To achieve this goal, the microstructural complexity and its evolution upon mechanical loading should be resolved by using, for example, *in-situ* electron microscopies (SEM, TEM), Raman microscopy, as well as advanced synchrotron radiation and neutron scattering techniques [8,9,266-271]. Multiscale modeling techniques could also be used to elucidate the microstructure-performance relationship with the assistance of statistical analysis of the high-throughput data thus produced [272]. Multiscale problems such as failure of materials, friction and load transfer between structures with atomistically smooth surfaces, flow and phase change of fluid with moving contact lines, and the dynamical processes in the bio-nano systems controlled by both the individual, molecular-level processes and their collective behaviors are the problems to be tackled.

Understanding mechanical processes at nanoscale could promote the development of nanotechnologies by proposing novel concepts of nano-devices. However, the scaling-up and amplification of device performance such as the power output of an actuator are critical for applications with practical interest, for which integrating nanostructures and their interfaces into macroscopic assemblies without sacrificing the significance endowed at nanoscale is crucial. For strain engineering [273], high-quality samples may be required to create high-level strain [41], and novel loading systems

should be developed to achieve desired distribution of strain states in the materials or structures [154,274,275]. One of the unique features of living system is their dynamical behavior as exemplified by the responsiveness, adaptiveness and self-healing abilities. Following the bio-inspiration, functional materials with dynamical mechanical responses could be designed [102,246,276-278]. Going beyond the conventional continuum mechanics framework built on equilibrium statistical mechanics, theory and models capturing the open and non-equilibrium characteristics of the living system at nanoscale is also a challenge remaining.

Finally, we hope the renovated concepts, theories and methods developed through the studies of micro- and nanoscale mechanical behaviors could drive the renaissance of mechanics as a bridging, quantitative discipline solving the complexity between fundamental physical laws and engineering applications [279], and as a driving force of technical innovation in a broader perspective.

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