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MESOMECHANICS: THE MICROSTRUCTURE–MECHANICS CONNECTION

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Abstract—Mesomechanics is a new research thrust to evolve non-continuum mechanics for heterogeneous materials. By fostering a closer collaboration between the materials sciences and the solid mechanics disciplines, this new thrust seeks to apply mechanics principles to the microstructural constituents of multiphase materials, thus placing the microstructure–mechanics relationship on a quantitative basis. This paper describes some of the challenges and opportunities that are brought forth by the study of mesomechanics.

INTRODUCTION

Structural mechanics evolved primarily from applied mathematics. Historically, the mechanician has assumed structural materials to be homogeneous and isotropic. Recently, the approaches have been modified to account for some anisotropy and some inhomogeneity. The materials discipline is an outgrowth of chemistry, involving processing to achieve desired material properties. The microscope enabled material scientists to study material microstructure and its relationship to mechanical properties. Major advances have been made in processing metals to achieve the desired microstructure and properties.

With the advent of engineered multiphase materials, most notably fiber composites, the prospect of designing material microstructure with specific properties presents a new opportunity as well as a new challenge for both solid mechanicians and material scientists. In fiber composites, for example, the fiber–matrix arrangement can be accurately controlled, making it possible to tailor the stiffness, strength and other relevant mechanical properties of the composite in order to meet prescribed functional requirements, and to mathematically describe these properties based on the principles of mechanics. It is expected that similar approaches can also be applied to engineered multiphase materials of other combinations of phase geometries and constituent types. The new trend is thus to consider the virtually unlimited possibilities of engineering a multitude of new materials such that they possess, *a priori*, properties which will respond with required precision, or will sustain service conditions in unusually severe environments.

This new trend has caused both the solid mechanics community and the materials community to re-examine their individual roles and their interrelationship. A much closer collaboration of the two communities is now necessary in order to quantitatively describe different classes of microstructures, to understand how a particular class of microstructure responds to loads and how it fails, to formulate appropriate constitutive relations, and to develop the processing necessary to obtain the desired microstructure. Drucker (1981) describes this trend as "...design of the microstructure to give any desired combination of...macroscopic properties". According to Salkind (1976), this concept of the design of materials is the real revolutionary impact of advanced composites.

During the past few years, several workshops, NSF (1984), ASME (1985), DARPA-ONR (1984), were conducted within the solid mechanics community, aimed at defining

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future directions for relevant research and advocating increased funding from the government. These activities have identified a wide range of solid mechanics problem areas for future research, involving materials in bioengineering, electronic, geological and structural applications. Common to all these problem areas, there is a need to relate material microstructure and its influence on macro-responses on a constitutive basis.

MESOMECHANICS: A RESEARCH INITIATIVE

The Air Force Office of Scientific Research has recognized that the recent advocacy of the solid mechanics community warrants a new research thrust and has responded with an initiative entitled: "Mesomechanics: the microstructure–mechanics connection" (Haritos *et al.*, 1987). A major goal of this research initiative is to establish, quantitatively, microstructure–property relationships based on principles of mechanics.

The new direction is prompted, in part, by the rapid acceptance of new materials, most notably composites. In the past two decades, composites usage increased from 2% in the F-15, to 10% in the F-18, to 30% in the AV-8B; and it is projected that the ATF (advanced tactical fighter) will contain 40–60% composites, according to Salkind (1986). These new structural materials have also been widely accepted by the commercial aircraft, automobile, sporting goods and machinery industries. Use of fiber composites will continue to expand based on reduced processing and material cost. Mechanics and material processing sciences are playing a closer role in composites, both in development and application.

Fiber composites represent but one class of multiphase materials engineered with designed microstructures. Other materials of current research interest include ceramics, ceramic and metal–matrix composites, chopped fiber and particulate composites, carbon–carbon and cementitious composites. It is certain that other multiphase materials with heretofore unimaginable microstructures will be developed to provide even greater stiffness and strength, to control acoustical and vibrational damping, or to improve resistance to impact loading and hostile environments.

The term "mesomechanics" is intended to describe an area of research that bridges the microstructure–property relationship of materials with non-continuum mechanics. This is in contrast to traditional approaches that develop constitutive models based on the behavior of phenomenological materials. Mesomechanics is aimed at developing the fundamental principles and the associated methodologies which can guide the creation of multiphase materials with the desired microstructure on one hand, and predict their in-service microscopic and macroscopic behaviors on the other.

The difficulties inherent in this new effort cannot be overstated. For what is proposed here will undoubtedly bring forth drastic modifications in the existing mechanics theories and, probably, new mechanics concepts. To go beyond the traditional concept of continua will require research innovations in both analytical and experimental mechanics.

NEW THRUSTS IN MECHANICS–MATERIALS RESEARCH

Against this background, the new research initiative will encompass fundamental studies in the following general areas.

Constitutive modeling of multiphase materials

The constitutive model is a mathematical representation of the deformation response of a material to externally applied loading, including environmental factors. The traditional continuum mechanics approach is to establish a set of mathematical relations linking the intrinsic stresses with deformation, i.e. strains. These relations are assumed to be uniformly valid for material bodies of arbitrary volume, implying that particle interaction is local or at an arbitrarily infinitesimal range. This assumption permits the concept of limit in differential calculus to be applied throughout the interior and on the boundary of the material body. The gradient and the divergence theorems, for example, are direct consequences of the continuum assumption (Fung, 1965). The necessary material smoothness thus makes it

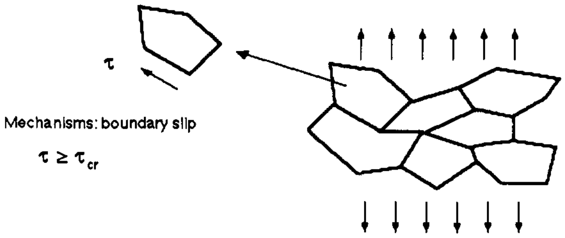


Fig. 1. A micromechanics model for polycrystalline solids, assuming grain boundary shear slip mechanisms (Lin and Ribeiro, 1981).

possible to derive a set of general constitutive relationships for a class of materials without inquiring into their material microstructure and micromechanisms of deformation.

The continuum assumption is, of course, no longer valid at the limiting microstructure scale. For most single phase metallic materials the limiting scale is likely to be of the order of the grain size; or, as in the case of a polymer, the size of the crystalline molecule. In multiphase materials, such as fiber composites, the limiting scale is of the order of the fiber diameter or layer thickness. Whatever the limiting scale, a thorough knowledge of the material microstructure and the micromechanisms of deformation is necessary in order to retain their important effects in a phenomenological description of material constitutive behavior.

For materials that exhibit inelastic behavior, for example, generalization of material constitutive behavior on the basis of the continuum assumption becomes difficult because the sources of inelasticity may stem from any of several possible microscopic deformation and damage mechanisms. Proper analysis of inelasticity will depend on the specific material microstructure and its interaction with loading. Past and present plasticity theories for metals have attempted to include material micromechanisms at the grain boundary level in the formulation of constitutive relations (Taylor, 1938; Bodner and Partom, 1975). In reality, however, empirical or semi-empirical approaches have usually been taken due to complexity of material microstructure and lack of understanding of the micromechanisms under loading.

Another example of the microstructural effect is residual stress which is known to be present in multiphase materials such as fiber-reinforced composites. Weitsman (1979), for instance, showed that curing variables can significantly alter the residual stress state in fiber-reinforced polymeric composites. To include the residual stress effect in predicting constitutive behavior, a direct approach would be to consider the material with its exact microstructure at the proper scale. Here, a micromechanics model of a highly redundant structure is required which must be analyzed with respect to the specific loading applied to it.

Figure 1 illustrates an example for such a micromechanics model by Lin and Ribeiro (1981) for the grain structure for a polycrystalline solid. The *in situ* properties of each grain are assumed known and the deformation of the solid is idealized as the result of a simple micromechanism identified here as continuous shear slip on one or more grain boundaries. Mathematically, the slip mechanism is described by a spring–dashpot model and the slip condition is provided by grain boundary shear strength, τ_{cr}. Hence, a progressive load–slip computation procedure based on a searching scheme can be devised which yields the desired load–deformation relationships. In principle, the scheme can calculate the microscopic stress fields in each grain and on its boundary at any time of loading or unloading, thus providing a basis for "material homogenization" to arrive directly at a material constitutive relation appropriate for the considered loading condition.

Such a "brute force" scheme for generating material constitutive relations that accounts for the effects of microstructure and micromechanisms is possible, though probably not practical, for highly complex multiphase materials with three-dimensional microstructures.

An alternative approach is to represent multiphase materials by a heterogeneous medium, the medium being endowed with "appropriate" effects of material microstructure and micromechanisms. To do so, sufficient detail at the microscale may still be needed in order to represent adequately these micro-effects in the material's constitutive relations.

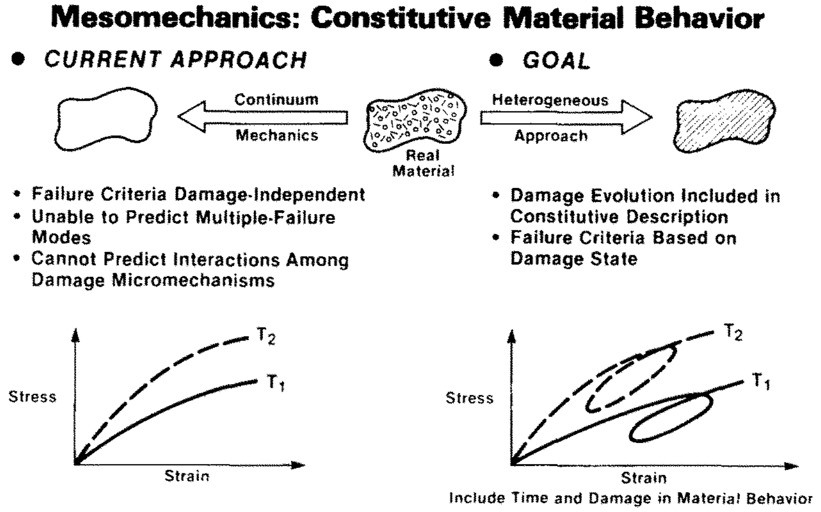


Fig. 2. Essence of mesomechanics: overcome the limitations inherent in the continuum approach and face the challenges inherent in the heterogeneous medium approach.

Thus, the developed approaches associated with the traditional continuum assumption will require major modifications.

Figure 2 depicts the essence of the continuum mechanics *vis-à-vis* the envisioned heterogeneous approach. While we identify in the former serious limitations, we also see in the latter formidable challenges.

A major challenge in mesomechanics is to mathematically describe the material microstructure—the complex shapes, orientations and distribution of the phases. This will serve as the common language used by the mechanicians and materials scientists alike. Figures 3(a)–(f) depict a sampling of a broad range of structural materials viewed on the dimensional scale of their property-determining microstructural features. Although these are two-dimensional sections, they nevertheless reveal the severity of the challenge. Quantitative microscopy or stereology, coupled with geometric probability concepts, has been used to relate material microstructure features, such as phase volume, surface area, integral curvature, intercepts, etc. with strength properties of metals (Underwood, 1970; Underwood and Banerji, 1986). In recent years, application of fractal geometry to characterize the morphology of the fracture surface of metals and ceramics opens up another possible avenue for developing generalized methods for qualitatively characterizing microstructures (Mandelbrot *et al.*, 1984; Mecholsky and Passoja, 1985). These approaches require further exploration, and the development of a common mathematical language for microstructure is the first major task for mechanicians and materials scientists.

A second challenge, perhaps the more difficult, is to link the kinematics of microstructural evolution with mechanics. Most of the work in relating the evolution of microstructures with thermodynamic forces has been in the field of metallurgy. For example, Taylor and Cahn (1986) showed that formation of a cusp in crystals can be mathematically related to the minimization of anisotropic surface energies. DeHoff (1984) connected the kinematics of the geometric cell structure of porous media with interfacial diffusion flux during the sintering process. From the mechanics perspective, however, linking the differential changes in microstructure with mechanical forces would seem to require considerably more understanding of the evolving loading and microstructure interaction mechanisms. As the microstructure and property characterization cannot be separated from the mechanics function in the overall structural response determination, relating microstructural evolution effects through material constitutive equations to mechanics theories is the real challenge of mesomechanics.

Damage mechanics of multiphase materials

Continuum mechanics failure theories are based on the stress state at a point. Plasticity theories allow description of a growing yield zone near areas of stress concentration.

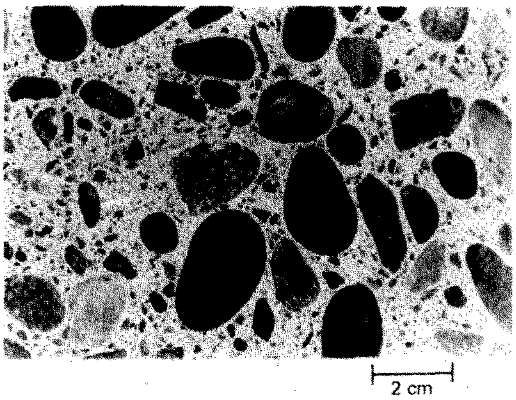


Fig. 3(a). Photomicrograph of plain concrete: aggregates (dark) in cement paste (light). Courtesy, Prentice-Hall (*Concrete: Structures, Properties and Materials*, 1986).

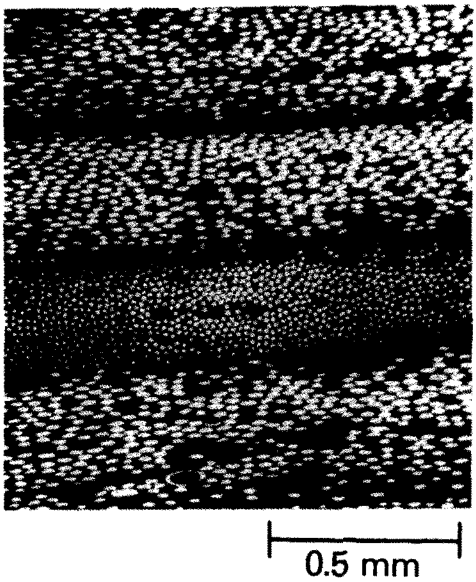


Fig. 3(b). Photomicrograph of a graphite–epoxy composite laminate: AS graphite fibers (light) in 3501 epoxy matrix (dark). Courtesy, ASM (*Metals Handbook*, Vol. 9, 1985).

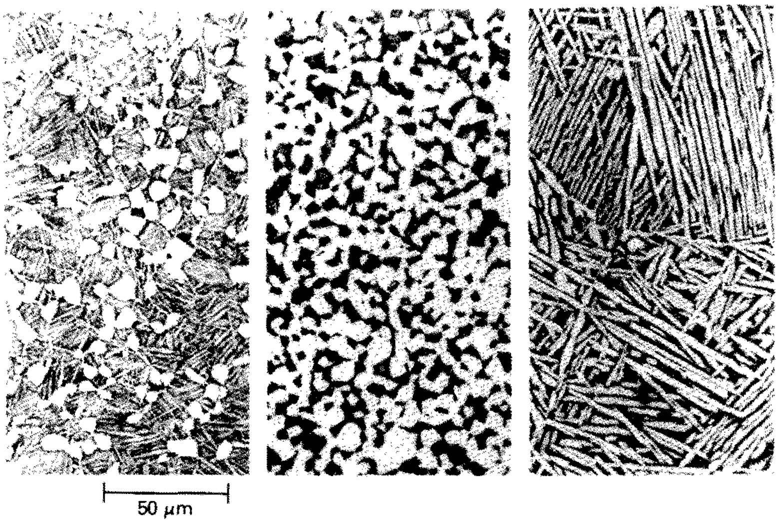


Fig. 3(c). Titanium alloy subject to three different processing conditions: alpha-phase (light) in beta-phase matrix (dark). Courtesy, *Scientific American*, Vol. 255, No. 4, p. 163, Oct. 1986.

Fig. 3(d). Eutectoid steel 1080: iron carbide (dark) in ferrite matrix (light). Courtesy, ASM (*Metals Handbook*, Vol. 9, 1985).

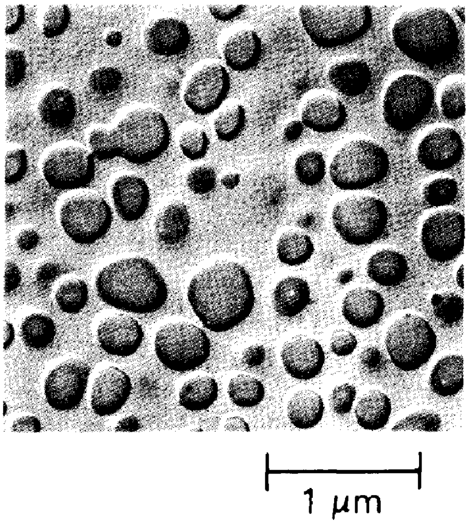


Fig. 3(e). IN-738 nickel-based superalloy: gamma prime particles in gamma matrix. Courtesy, ASM (*Metals Handbook*, Vol. 9, 1985).

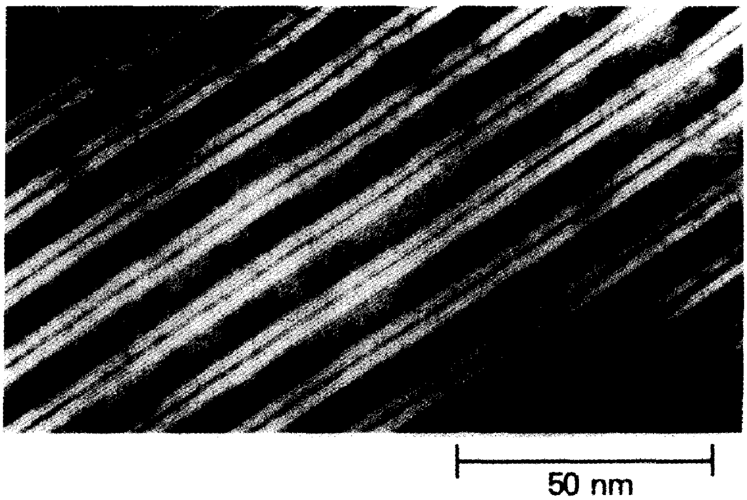


Fig. 3(f). Three-layer zinc–manganese–selenium super lattice built by molecular beam epitaxy. Courtesy, *Scientific American*, Vol. 255, No. 4, p. 134, Oct. 1986.

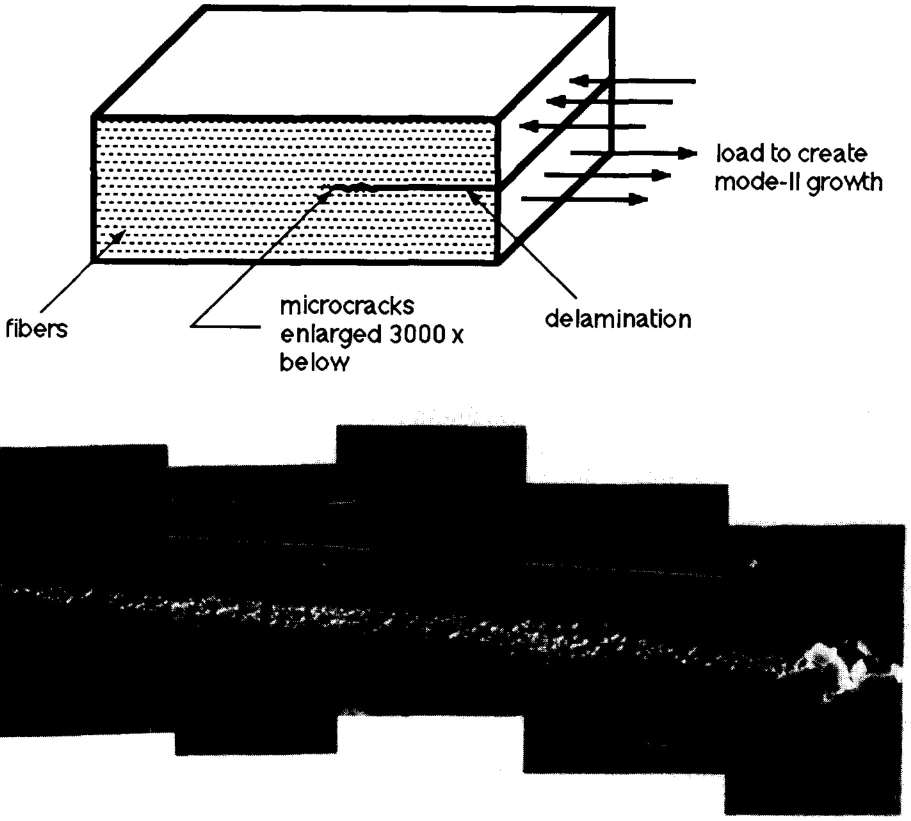


Fig. 4. Microcracks in the fiber–matrix interface formed ahead of delamination. Specimen is unidirectional graphite–epoxy loaded in mode-II fracture (Corleto *et al.*, 1987).

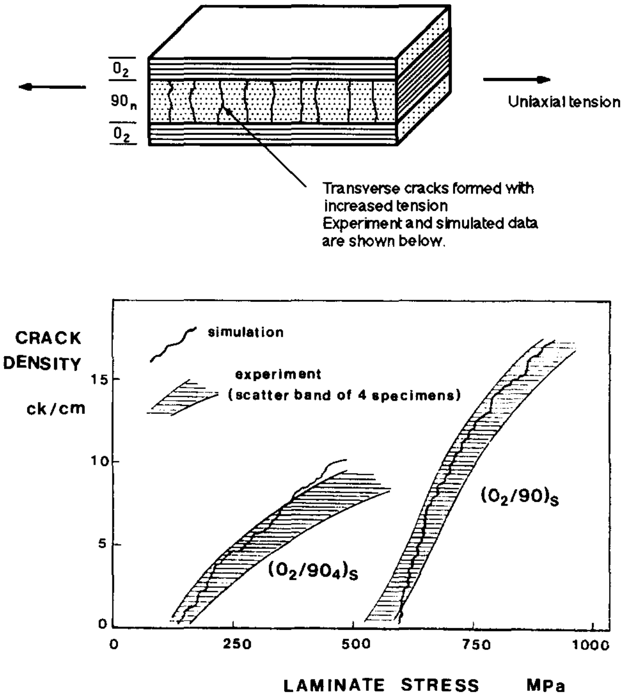
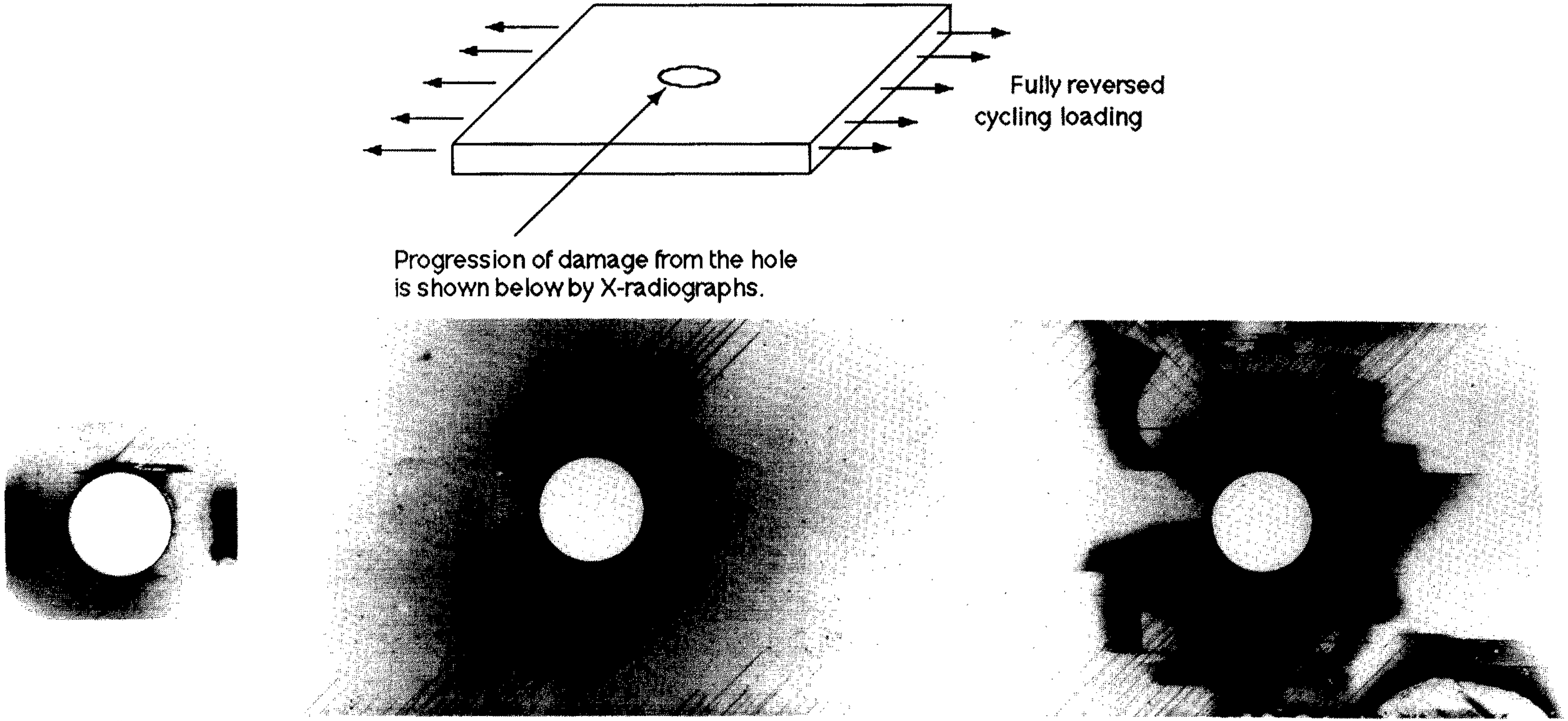


Fig. 5. Development of 90°-layer transverse cracks in graphite–epoxy $[0_2/90_n]_s$ laminates. Simulation model is based on an assumption of distributed effective flaws in the 90°-ply (Wang, 1984).



~200 Cycles ~5,000 Cycles 10,000 Cycles

Fig. 6. Progression of damage at early life, middle life and impending failure. Specimen is graphite–epoxy $[(0/45/90/-45)_s]_4$ loaded in tension–compression fatigue (Reifsnider and Bakis, 1986).

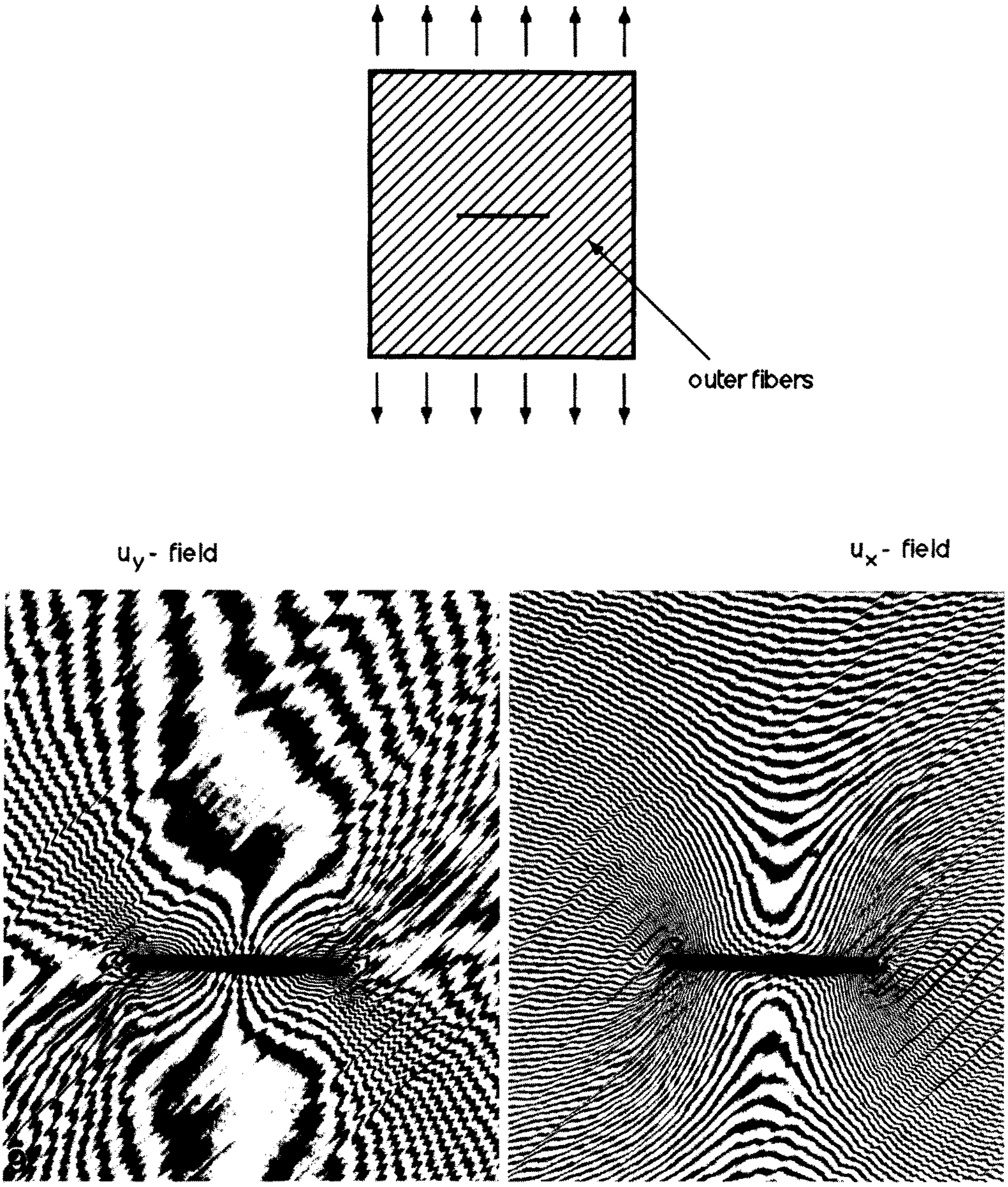


Fig. 9. Moire-displacement fields showing distorted fringe patterns by subsurface microstructure. Specimen is a notched $[\pm 45/0_2]_s$ B/A laminate loaded in tension (Post, 1987).

Dislocation theories provide identification of weak slip lines or slip surfaces in materials that fail in shear. Fracture mechanics theories follow the crack tip and its propagation trajectory. These failure theories treat local effects from a phenomenological point of view and require a physically-based stability or instability criterion, separated from the material constitutive relations. In recent years, the concept of continuum damage by Kachanov (1986) has come to include damage as a state variable in the material constitutive relations (Bodner and Chan, 1986).

With multiphase materials, new concepts of material failure are needed in order to account for the generic factors at the phase scale. One important factor is interface bonding between material phases. Experience with fiber composites (Salkind, 1968) has shown that fiber matrix interface bonding can be manipulated to change the initiation and coalescence mechanisms of microcracks and to yield a wide range of values for the apparent material toughness and other macro-properties. Figure 4 shows the formation of a string of microcracks in the matrix ahead of a delamination crack at the fiber–matrix interface in a unidirectional graphite–epoxy composite under mode-II fracture condition. Corleto *et al.* (1987) suggested that these microcracks represent a major source of strain energy dissipation during delamination growth; but that the microcracking mechanisms, the actual formation processes and their relations with the fiber–matrix interface properties are not fully known. On the phenomenological level, delamination fracture of this kind could not be realistically modelled.

Another factor is the apparent randomness at the phase scale. Microcracks in composites have been observed to occur randomly under macroscopically homogeneous stressing conditions, which leads to statistically distributed failures and failure modes (Harrison and Bader, 1983). Reifsnider and Highsmith (1981) showed that development of these distributed microcracks is, on the other hand, regulated intrinsically by the geometry of the material microstructure.

An example is shown in Fig. 5, where a graphite–epoxy cross-plied laminate is loaded in axial tension. Under increasing tensile loading, the inner 90°-layer can suffer multiple cracks orientated normal to the load. The formation of these 90°-layer cracks occurs before any other modes of damage, such as delamination or fiber breaking. The evolving nature of these cracks with relation to the applied tension is seen to vary with the thickness of the inner 90°-layer. The simulation was provided by a fracture model due to Wang (1984) based on assumed material flaw distribution in the material ply and an account for the effects of the laminate microstructure.

In general, microcracking or damage development in multiphase materials is a process that evolves with load, space and time. Instability of the evolving process usually determines the apparent material failure at the macroscale. Figure 6 shows an example due to Reifsnider and Bakis (1986). Here, the progression of damage in a composite laminate having a small through-hole is shown by x-radiographs taken at three stages of fatigue loading. The damage is seen to develop from the hole boundary in the form of matrix cracks and delaminations. These then grow stably with fatigue cycles. The pattern of growth, the growth rate and the critical growth that leads to instability failure are all influenced by the laminate microstructural arrangement. To describe processes of this kind and to establish a general criterion for instability would seem to require a combined statistical and micromechanics approach.

Stress waves and dynamic responses

Applications of stress wave propagation include a wide range of scales from earthquake monitoring to material micro-defect detection. Theories describing wave motions in solid bodies have largely been developed on the basis of continuum mechanics, such as found in the text of Kolsky (1963). Constitutive theories, which are formulated within the confines of the continuum assumption but include effects of material inhomogeneity, have been advanced primarily for stress waves in oriented media (Eringen, 1976). With multiphase materials, however, new approaches for such phenomena as non-linear dispersion, energy dissipation, multiple scattering and surface wave effects will be needed for stress wavelengths comparable to the characteristic dimensions of the phases. Any such endeavor would require an iterative approach in which the character of the sources, the *in situ* mechanical properties of the material phases, the inherent microstructure, and micromechanisms are related. Correlative studies involving analytical or numerical simulation based on non-continuum constitutive relations and experimental measurement of responses at both the phase scale and the overall structural scale are needed in order to properly delineate the true nature of the stress waves propagating in multiphase materials.

A related challenge is to understand the mechanics of stress wave-induced damage, such as spalling in materials subjected to impact loading. As depicted schematically in Fig. 7, the phenomenon of spalling involves both global (vibration) and local (stress wave propagation) responses and their interactions. Research in the areas of impact dynamics and dynamic fracture have gained wide interest in modern times (Goldsmith, 1960; Williams and Knauss, 1985). Much more remains to be investigated in the context of mesomechanics, however.

Very high temperature behavior

There is an increasing demand for structural materials to function under very high temperature conditions and for prolonged duration. The wing skin of the hypersonic transport of the future, for example, must be able to retain its stiffness, strength, dimensional stability and other properties during long flights at 2000°F or more. Future turbine engine components will have to operate at even higher temperatures. New material systems such as ceramic composites and intermetallics have the potential for satisfying these stringent requirements.

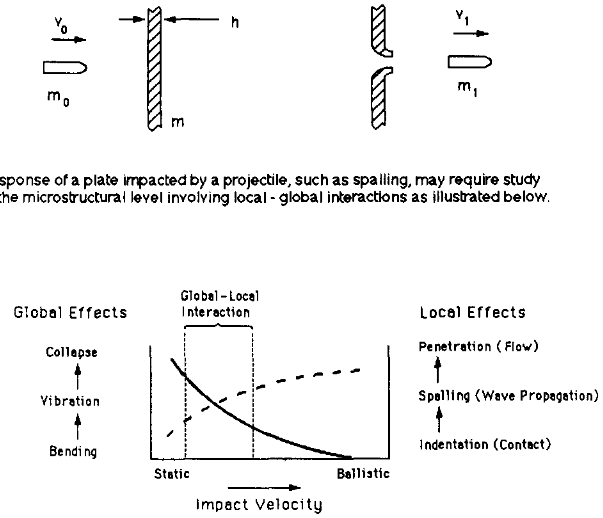
The mechanics of these special materials is in an embryonic state of development even at the phenomenological level. Some progress has been made in modifying existing mechanics methods to accommodate the new phenomena. For example, the principles of thermoelasticity for isotropic materials have been extended to composites and other anisotropic materials, and to inelastic states of deformation by Dvorak and Wung (1984); phenomenologically-derived constitutive theories have incorporated temperature effects through internal variable provisions by Aboudi (1985) and Rubin (1986).

Shahinian and Sadananda (1976) studied crack growth in IN-718 alloy due to high temperature fatigue and creep and found that the conventional linear rule for cumulative damage could not account for apparent load-sequence effects. Figure 8 shows an example. Here, the IN-718 specimen with a pre-crack was tested at 1200°F where the specimen was first loaded in tension to a peak load and held for a period of time; it was then followed by cyclic fatigue with the same maximum peak load. Apparently, the initial hold-time allowed creep deformation and possibly changed the microstructure near the crack-tip. This caused the subsequent fatigue crack growth rate ($\mathrm{d}a/\mathrm{d}N$) to be significantly influenced by the initial hold-time. In this case, crack growth predictions could not be based on some simple cumulative damage rule as interactions between the creep and fatigue damage mechanisms could not be accounted for in the model.

Most of the current understanding of high temperature material behavior is restricted to simple loading conditions (e.g. one-dimensional creep) and thus lacks general applicability. A deeper understanding of thermomechanical deformation and damage that occur at the scale of material microstructure is needed in order to construct micromechanics models that can account for transient, high rate and multi-directional thermomechanical loads.

Experimentation to identify the underlying mechanisms of thermomechanical response is a major challenge due to difficulties posed by the hostile environment. Instruments for making *in situ* measurements at the microstructural scale are now lacking both in numbers and in precision. Nevertheless, efforts in this direction must accompany any development of advanced constitutive models that incorporate microstructural and damage effects.

The consequences of microstructural evolution in response to high temperature loading, including material property change and damage accumulation (such as evidenced in creep rupture and thermal fatigue) need to be studied in order to provide a reliable basis for failure criteria, and for synthesizing materials with tailored microstructure to achieve desired high temperature performance properties.



Response of a plate impacted by a projectile, such as spalling, may require study at the microstructural level involving local - global interactions as illustrated below.

Fig. 7. Schematic illustration of dominance of the global (solid line) and local (dashed line) effects in structural plates impacted by a projectile. Region of global–local interaction occurs within a specific range of impact velocities.

Non-linear structural behavior

The mechanics of multiphase materials is inherently nonlinear. The immediate consequence of nonlinearity is the loss of the applicability of the superposition principle. The response to multiple loading or excitation conditions cannot be synthesized from the individual effects of each condition by simple addition. Another consequence of nonlinearity is the multiplicity of possible equilibrium configurations for a given set of operational conditions with varying degrees of stability attributes.

Both consequences have serious implications for all aspects of material synthesis and application. From a material characterization standpoint, non-linear scale (size) effects

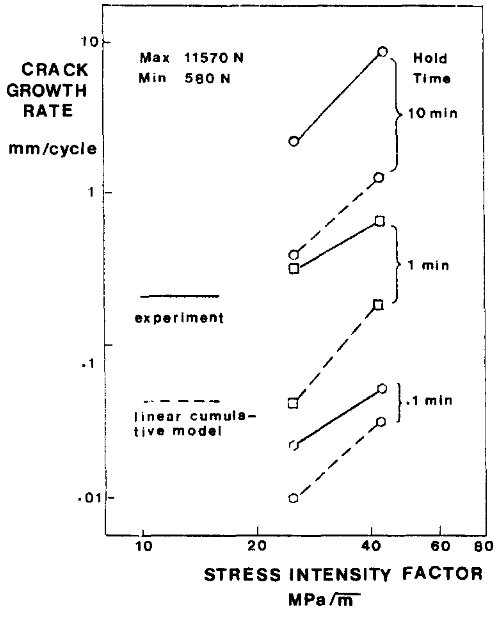


Fig. 8. Effect of hold-time (creep) on fatigue crack growth rate of IN-718 alloy tested at 1200°F. Calculated results (dashed lines) are based on linear cumulative damage rule (Shahinian and Sadananda, 1976).

must be considered in extrapolating test data or measurements from small size coupons to large components; or from simple loading to complex loading conditions. Load sequencing effects must be understood if complicated dynamic, thermal, and other time-dependent loads are to be amenable to analysis within the context of mesomechanics.

The stability implication of non-linear behavior of multiphase materials in engineering structural systems opens another area of fundamental research. Recent studies of chaotic motion in geometrically non-linear systems have identified behavior that has no counterpart in linear systems (Thompson and Stuwart, 1986); chaotic motion has also been shown to occur in systems subjected to deterministic excitations, devoid of any random input (Moon, 1980). With multiphase materials, local non-linear responses of a constitutive origin, such as those manifested phenomenologically in hysteresis, strain hardening, relaxation and creep, must be examined from the viewpoint of total structural system stability.

Computational and experimental mechanics

The problems to be studied in mesomechanics will generally be nonlinear, time dependent and three-dimensional in nature. Mathematical solutions to these problems pose an unprecedented challenge for computational mechanics. Even with the availability of high-speed supercomputers equipped with parallel-processor architecture, it may still be impractical to perform the analyses and simulations defined within the context of mesomechanics in the near future.

Although extensive research and development of modern computational methods has been conducted in non-linear structural and solid mechanics in recent years, problems persist in accurately computing the true and complete non-linear solutions (Noor and McComb, 1980; Noor and Atluri, 1987). In finite element applications, for example, mesh refinement to improve numerical precision may compromise the inherent non-linear effects accompanying the physical system. It seems that any future development of computational methods must involve insightful modeling, keenly related to the physics of the micromechanisms which are to be simulated.

The physical quantities to be detected and measured must be resolved at a wide range of dimensional scales. For many multiphase materials, measurement in the micrometer and submicrometer scales may be necessary to resolve changes in microstructure. Recent advances in Moire interferometry, for instance, have enabled observation of high-gradient strain fields complicated by sub-surface microstructure in fiber composites. Figure 9 is an example due to Post (1987) which shows the Moire displacement fields taken from a boron–aluminum composite laminate with $[\pm 45/0_2]_s$ construction. Sharp distortion of the fringe patterns near the central slit is caused by local strain variation due to fiber–matrix interaction in the outer 45°-layer.

Clearly, innovative instrumentation and testing techniques are needed to measure the desired quantity at the microscale, nondestructively, in real-time, by remote sensing as well as by *in situ* monitoring. The high precision required, the very short response time and the hostile testing environment in which measurements are to be made, all require novel developments in experimental mechanics.

CONCLUDING REMARKS

In this paper, we have endeavored to outline areas proposed for increased emphasis in future structures and materials research. It is clear that, more than ever before, it will be necessary for the mechanician and the materials scientist to join efforts and perform as a team. The task will require repeated and refined correlations between physical understanding and mathematical description for the phenomena under consideration. This will be a major challenge to both communities. At the same time, we believe that the research areas outlined in this paper represent examples of the emerging field of mesomechanics, a field which presents major opportunities for future progress in materials and structures technology.

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