Particle and Continuum Aspects of Mesomechanics

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George C. Sih
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The International Society of Mesomechanics (ISM) was established in 1996 to foster the advancement of science and technology in relation to segmentation of scaling in size and time where transitory behavior is created. For each succeeding year, the mission of ISM becomes better focused. The 9th annual meeting Meso 2007, “Particle and Continuum Aspects of Mesomechanics: Integrity Thresholds for Materials and Structures”, May 13-17, was held at Presqu’ile de Giens in the south of France, its aim being to disseminate the current thinking on the subject to the scientific and engineering community at large.

It is becoming clear that materials and structures undergo a hierarchy of thresholds at the different scale, although not all of them could be readily identified. The assessment depends on the size of region under consideration and the resolution of the microscopic or telescopic site. The birth and death of organic or inorganic matters are manifestation of thresholds representing the transitory character of nature. As the body size becomes smaller and smaller, these thresholds are less obvious and there are no reasons why they should disappear, although the physical laws governing their behavior may differ. Still a matter of debate is the appropriate use of the bulk properties as an average or of the local properties of discrete particles. Mesoscopic regions prevail where the particle and the bulk interplay. The mesoscopic behavior may be loosely regarded as the transition from particle to continuum or vice versa. This transition is no doubt size and time scale size sensitive. Reconciliation of the contrasting views are to say the least not in sight.
The present indication is that physical laws are not size scale invariant. Hence, multiscaling is not only an issue of measurements but it embarks on the foundation of physics, chemistry and mechanics. What has already transpired and has yet to be developed may not be a continuous process. Segmentation of size and time scales can be found in the distinction of macro-stress, micro-stress and dislocation-stress as they are identified with the corresponding linear dimension of the constituent of the solid. They can be ranked with the respective units of MPa, GPa and EPa. The range of scaling, however, appears to be truncated with the intermediate units of TPa and PPa missing. They can presumably (but not necessarily) correspond to a cluster of dislocations and subgrain boundary precipitates with linear dimensions of the order of $10^{-6.5}$ cm and $10^{-5.0}$ cm, respectively. This completes the full range of defects ranked by the linear dimension from $10^{-2.0}$ cm to $10^{+8.0}$ cm and the corresponding stresses with units of MPa, GPa, TPa, PPa and EPa, such that their differences are separated by three orders of magnitude in Pascal. By the same token, similar features of size scaling can be found by observing larger objects that are cosmic in size. If a particle size of $10^{-32}$ cm in linear dimension is used for reference, then the universe, galaxy, solar system and earth would follow the respective dimensions of $10^{38}$, $10^{23}$, $10^{13}$ and $10^{8}$ cm. This corresponds to $10^{80}$, $10^{65}$, $10^{55}$ and $10^{50}$ particles. The same particle size, however, will not yield a reasonable size spectrum for objects smaller than the human body. This observation suggests a discontinuity in the process of scaling, not to mention an inability to account for the reconciliation of the difference between the discrete and continuum viewpoints.

These mind boggling problems will remain for times to come. Nevertheless, it is important to be aware of their implications. The topics selected for Meso 2007 will perhaps help to illustrate the relation of thresholds to multiscaling. Among the topics suggested are:

- Flow through capillary tubes in contrast to pipes
- Laminar and turbulent flow transition
- Heat convection of thin wire in contrast to cylinders
- Electrical conductance of macro- and nano-circuits
- Rubbery and glassy polymers
- Single- and poly-crystal behavior
- Strength of wires and round cylindrical bars
- Uni-axial and multi-axial material: linear and non-linear response
- Thin and thick plate behavior
• Brittle and ductile fracture
• Small and large crack growth behavior
• Low and high temperature effects
• Local and global material property characteristics
• Small and large bodies: size and time effects
• Specimen and structure

It should also be mentioned in passing that finding a common ground for life and material science may generate new ideas that are needed to unravel the secret of nature. Mesoscopic behavior seems to be entangled with transition that necessitates the notion of thresholds.

The encouragement and support provided by the sponsored are gratefully acknowledged:

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The efforts of the contributing authors and those who assisted in organizing the conference are gratefully acknowledged. Special thanks are due to the members of the local committee for taking care of the participants.

Presqu’ile de Giens, France
May, 2007

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SECTION I

Physical Mechanisms of Multiple Damage
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Multiple Hierarchical Scale-Dependency on Physical Mechanisms of Material Damage: Macromechanical, Microstructural and Nanochemical

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ABSTRACT: The evolution of nature entails a scaled time/size process whereby matters are known to be made of minute entities that gradually build up into larger and larger conglomerates. The forces that bond these constituents together have intrigued solid state physicists to invoke interatomic and intermolecular models for the study of the strength of materials and/or their breaking strength. In particular, fracture mechanics seem to have revealed a hierarchy of relationship between scale size and physics that can be best referred to as “macromechanical” and “microstructural” at the macro and micro scale, respectively. That is to say macroscopic damage appears to be inherent with the release of mechanical energy while microscopic defects are typified by the microstructural details. By the same token, chemical effects are intimately related to the behavior of atoms at the nanoscale that can be described simply as “nanochemical”. These three classifications coincide with the regions I, II and III that below the threshold portion. They have been commonly referred to for the fatigue crack growth data of metals. In light of the scale/size-physics character of material damage, a reinterpretation of fatigue data is in order. A common ground may be established for addressing the disorder of systems related to material, chemical, biological and neurological science, not excluding the possibility of future considerations for “picobiological” and “femtoepigenetical” effects.

The development of the generalized multiscale model may start by exploring data for the fatigue damage of metals and polymers and including the transitory behavior of micro- and macro-cracking. Variability in size, time and material is allowed to test the versatility of the model for connecting the micro and macro results. This can lead to a better understanding of why small bodies do not behave the same way as the larger bodies. To this end, a dual scale micro/macro line crack model will be used to show that the scale transition sensitive quantity $\Delta K_{\text{macro}}$ can reinterpret the existing fatigue data for metals and polymers making them size insensitive. More simply put, the sigmoidal curve can be transformed to a straight line and there is no longer the need to distinguish the difference among the three regions I, II and III.
Three essential parameters are found in the formulation; they are used to adjust the crack surface tightness \( \sigma^* \) (loading), the micro/macro material properties \( \mu^* \) and characteristic length \( d^* \), the last of which is related to the small opening segment of the microcrack tip. This unique feature differentiates the modeling of microcracks from the macrocracks. A key observation of fatigue striations from micrographs is that the microcrack tip always remains open. Damage due to crazing/cracking at the end of a microcrack in polymer is assumed to be qualitatively the same as that for a metal. That is craze initiation by microvoid nucleation may be comparable to void initiation in metals. Therefore, the invocation of a small opening segment with characteristic length \( d^* \) similar to that for metals is plausible. In this way, the micro-macro-crack transitory behavior will be examined for fatigue crack growth in the 2024-T3 aluminum and polyvinylchloride (PVC). Aside from the disparities in the applied loads, similarities of the fatigue crack growth behavior for the two different materials are noted from the viewpoint of multiscaling. Linearization of the fatigue data encourages the further extension of the model to include nano effects.

**KEY WORDS:** Microcracking, macrocracking, transition, size-time interaction, macomechanical, microstructural, nanochemical, metals, polymers, fracture, crazing, microvoids, fatigue, characteristic length, tip opening, form invariant, multiscaling
1. Introduction

The fracture of solids has intrigued scientists since the days of Galileo by testing for the strength of wires to that of beams. Fracture mechanics became popular as a discipline that provided a means to inspect and control possible failure of structures such as air transports, nuclear reactor components and ship sub-structures. This pursuit of knowledge related to the breaking of materials embarks on understanding the basic constituents of matter and energy. It is no different than modern high energy particle accelerators that probe deep into the atom hoping to unravel the connections among the elementary particles. Two basic parameters that stand out are the impact energy and the corresponding length dimension characterizing the size of electron, proton, neutron, muon and so forth. Scaling of the particle size and the corresponding energy in GeV, TeV, etc. are the means to establish an order for ranking based on the energy density. This same approach has been used at the macroscopic, microscopic and mesoscopic scale (Sih et al., 2006b; Sih et al., 2004a; Tang et al., 2005) such that the results at the different size and time scales can be connected for the development of multiscale material damage models (Sih et al., 2005; Sih, 2006a; Sih et al., 2007b).

Test data collected on the fatigue of metals for the past three decades have revealed that they naturally fall into three distinct groups according to use specificity. Systematic investigation of macro-size cracks were prompted by the aircraft industry for testing the strength of aluminum thin sheets with preexisting through cracks. Up to this date the sigmoidally-shaped crack growth rate curves consisting of regions I, II and III remain as the landmark in the field. Microscopic studies of crack initiation for smooth specimens under fatigue have centered on crack growth from the specimen surface. Intergranular and/or transgranular embedded (or interior) cracks have been associated with the effects of stress corrosion where chemistry effects are of primary interest. Each of these three categories of material damage by fatigue has been well recognized but their inter-relations are still left open even though regions I and II of the two-parameter (Paris, 1962) crack growth rate curve are known to involve the transition of surface to through cracks, or more precisely microcracks to macrocracks. Reconciliation of this transitory behavior appears to be opposed by the disparities of the geometry of surface and through cracks, not to mention the nanocracks which are completely engulfed within the material. In this respect, their equivalency may require the approach of particle physics where the state of all bodies large or small are ranked by the energy (or density) level and the corresponding characteristic length (Sih, 2006c).

What needs to be emphasized is that the multiscale process of fatigue can be resolved fundamentally head on by considering the non-equilibrium character of cumulative energy dissipation from damage. Preliminary work (Sih et al., 2004b; Sih et al., 2004c) has calculated the hysteresis energy dissipation using the isoenergy density theory (Sih, 1988). The accuracy of prediction can be enhanced by the application of high speed and high memory micro-processors that are now available.
However, there are still considerable time gaps between the current “Fracture Control” procedure and the use of large scale computations. Cyberinfrastructure (Atkins, 2003) advocated by NSF for engineering education and research is a step closer to the control of material and structure failure in the cyberspace. In the meantime, enhancement can be made to improve the existing models, but not at the expense of abolishing the state-of-the-art of fracture control. It is in this spirit that the following work will be presented.

2. Linearization of two parameter fatigue crack growth relation

The basic premise of chemistry and physics is that all matters share the common building blocks. They should be reducible to a few being common to all. Such a hypothesis seems reasonable but it can neither be proved nor validated. The study of fatigue crack growth for metals seems to follow the same route. It started with the two parameter relation

$$\frac{da}{dN} = C(AK)^n$$

in the 1960s (Paris, 1962) and gradually slipped into the investigation of smaller and smaller cracks in the 1990s (Vasudevan et al., 1994; McDowell, 1997; Vasudevan et al., 2001; Newman Jr. et al., 2004; Jones et al., 2004; Noroozi et al., 2005; Jones et al., 2006). The order of magnitude crack size “a” reduced from about $10^{-1}$–10 mm to $10^{-2}$ mm or smaller. The precise representation of the single geometric parameter “a” for the crack size that may be more than one dimensional remains unclear. Most recent works delve into the previously referred “threshold” zone known as region I that is beyond the validity and/or application of Eq. (1). Nevertheless, the transition from region I to II within which Eq. (1) is assumed to be valid has been the subject of discussion for more than three decades. Despite the criticisms of Eq. (1), it still plays the central role of the current “Fracture Control Methodology” that is adopted by the FAA (Federal Aviation Agency) and NRA (Nuclear Regulatory Agency) for regulating the inspection and maintenance of aircrafts and nuclear reactors, respectively. Such a trend is not likely to change in the near future as mentioned earlier. More specifically, The simplicity of the straight line relation of Eq. (1) with C and n being the respective y-intercept and the slope as shown in Fig. 1(a) has overwhelmed the majority. For the 2024-T3 and 7075-T6 aluminum in (Broek et al., 1963) C and n can be determined from pre-cracked panels with the corresponding half-crack length a as indicated in Fig. 1(b). Note that the micro/macro transition zone corresponds approximately to $a = 1$-10 mm below which is the zone of microcrack propagation that the data in (Broek et al., 1963) will not apply. Micro- and nano-cracks, however, are the interest of those attempting to understand microscopic and nanoscopic damage. One of the key issues is that whether linearization can be extended to region I in Figs. 1 or even smaller size scales? That is to say though the crack length data in Fig. 2(a) can be divided into different scales identified with regions I, II and III, it is not obvious that the two-parameter formalism of Eq. (1) can be
extended to regions I and III as indicated in Fig. 2(b) such that the transient zones would disappear. Obviously, the constants B and m in

$$\frac{da}{dN} = B(\Delta K_{\text{macro}})^m$$

(2)

would differ in addition to the fact that $\Delta K_{\text{macro}}$ is no longer the same as $\Delta K$ in Eq. (1). The foregoing proposition may seem trivial but it enables linear interpolation of the results from micro to macro or perhaps even to nano.

(a) Fatigue curve for metals

(b) Crack size segments for aluminum

Figure 1. Two-parameter representation of fatigue crack growth rate for metals

(a) Crack length: nano→macro

(b) Crack growth: nano→macro

Figure 2. Data for crack length and growth connecting nano→micro→macro
3. Dual scale micro-/macro-cracking model

Micro-/macro-cracking behavior (Sih et al., 2006b; Sih et al., 2004a; Tang et al., 2005) has been examined with emphases placed on the differing physical mechanisms as the scale changes. The typical macrocrack corresponds to two free crack surfaces specified by the free-free boundary conditions that are well known. More fundamental is the macrocrack tip stress singularity with the order $r^{-0.5}$ where $r$ is the distance from the singular point. The same order of macrostress singularity also prevails for the traction-traction boundary conditions. Hence, the condition of free-free crack surface is not unique. The irregular nature of the microcrack is exemplified by the constant opening of the tip region. This special character of the microcrack tip has been observed from micrographs of fatigue striations in (Molent et al., 2006) for the aluminum alloy. A schematic of the situation is shown in Fig. 3(a) for a centered crack of length $2a$ with one-half symmetry. The body is under tensile and compressive reversal loading. The tip region of length $d$ is microscopic in Fig. 3(a) and is enlarged in Fig. 3(b). The quantity $\sigma_0$ stands for the restraining stress that is inherent of the resistance of the material to close the crack in addition to the fact that a macrocrack can close under compression and become a microcrack while a microcrack can open and become a macrocrack. It is the opening distance that dictates the scale size of the crack and not the length. To be kept in mind is that the use of the stress intensity factor $\sigma \sqrt{\pi a}$ in LEFM (linear elastic fracture mechanics) must be qualified by the crack length to the finite crack tip curvature relation. This has often eluded the attention of the user. In practice, the crack length alone cannot be the deciding factor regardless of whether the crack is micro or macro.

Hence, no a priori assumption should be required of the scale classification of crack growth in fatigue. But rather the decision depends on the interpretation of $\Delta K_{\text{macro}}^{\text{micro}}$ in Eq. (2). More precisely, the expression for $\Delta K_{\text{macro}}^{\text{micro}}$ will account for the transition behavior of micro-/macro-cracks.

3.1 Microcrack intensification

Consider the crack configuration in Fig. 3(a) where the panel is pre-cracked and assumed to coincide with those tested in (Broek et al., 1963) for both the 2024-T3 and 7075-T6 aluminum alloys. Their mechanical properties are given in Table 1. An initial notch about 1 mm deep and 0.2 mm wide is introduced by using a jeweler saw. The specimens are then fatigued to produce two natural fine line cracks at both ends of the saw cut. The natural cracks are tightly closed and not readily visible. Contact stresses prevail on the crack surfaces must therefore be accounted for in the derivation of $\Delta K_{\text{macro}}^{\text{micro}}$. Modeling of the open microcrack tip segment as illustrated in Fig. 3(b) is motivated by the observation in (Molent et al., 2006). A mixed boundary condition is taken for expedience although this representation is by no