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14. ABSTRACT This report summarizes the progress made in developing the theoretical underpinnings for two new theories of brittle fracture. One is based upon an extension of continuum mechanics to the nano-scale while the second is based upon a strain limited constitutive relation. In contrast to classical fracture theories, the new theories predict bounded crack tip stresses and strains. The first theory is implemented by including classical bulk properties with a novel boundary condition arising from the jump momentum balance enforced on fracture surfaces which are modeled as dividing surfaces with excess physical properties including surface free energy, surface tension and surface entropy. In the second, classical boundary conditions are applied to novel bulk constitutive relations. As a result of the bounded crack tip stresses and strains, it was necessary to introduce a new notion of crack tip Energy Release Rate (ERR) and a new fracture criterion.					
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FINAL TECHNICAL REPORT

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Title: Modeling Interfaces through an Extension of Continuum Mechanics to the Nanoscale with Application to Fracture, Debonding and Composites

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PRINCIPLE INVESTIGATOR: Jay R. Walton

A central issue in the use of advanced materials in structural applications is their susceptibility to catastrophic failure due to fracture. Being able to predict when cracks will form, and when and how they will propagate is crucial to predicting material reliability in a service environment.

Classical linear elastic fracture mechanics (LEFM) has been utilized successfully for predicting crack initiation and quasi-static (slow) crack growth in many brittle structural materials. However, it has been shown to be inadequate when attempts are made to apply it in simplistic fashion under other situations such as to materials exhibiting significant ductility or viscoelasticity, or to cracks propagating dynamically (even in brittle materials), or to fatigue cracking. Moreover, as a physical theory, LEFM has a well known internal inconsistency. Namely, it is predicated upon the assumption of infinitesimal strains while simultaneously predicting strain and stress singularities at a fracture edge. Singular stresses and strains are predicted even when the theory is generalized to the nonlinear setting of finite elasticity. Additionally, LEFM predicts blunt crack tip opening profiles while experimental observation suggests crack tips should have sharp, cusp-shaped profiles.

Various strategies to circumvent this internal inconsistency of LEFM have been explored over the past fifty years, but few of them have explored the fundamental role that nanoscale, interfacial physics plays in understanding the mechanics of the region surrounding a crack edge. A central goal of the research effort has been to exploit in a variety of fracture scenarios a novel approach to modeling brittle fracture in the context of continuum mechanics recently introduced by the Principal Investigators (PIs) that incorporates critical interfacial effects through viewing fracture surfaces as “dividing surfaces”, in the sense of Gibbs, endowed with physical properties such as internal energy, entropy and surface stresses.

A primary objective of the proposed research was the formulation and combined analytical and numerical solution of a variety of canonical fracture and other interfacial boundary value problems. As that work progressed, it became evident that a new theoretical foundation for an energy based fracture criterion was required as well as a rigorous analysis of the fracture boundary value problem. This task consumed most of the initial effort of the final grant and resulted in a new definition of the Energy Release Rate (ERR) and substantial progress towards developing an elegant new theory of its use as a fracture criterion along with a rigorous analysis of the corresponding analog within the new fracture theory of the canonical Griffith crack problem. Subsequently, the technologically important and much more difficult extension of the theory to interfacial fracture was undertaken.

In the final year of the grant, an entirely new approach to modeling fracture based upon the premise that the logical inconsistencies of classical LEFM could be avoided by introducing a strain limiting constitutive relation for the bulk material behavior while keeping the classical idealized fracture boundary conditions. This approach contrasts with the previous one in which the classical idealized fracture boundary conditions are modified to reflect viewing fracture surfaces as dividing surfaces while keeping classical linear elastic bulk material behavior. It was shown in the setting of a single anti-plane shear crack in homogeneous material that this second

approach also predicts continuous, nonsingular crack-tip stress and strain thereby avoiding the logical inconsistencies of classical LEFM. What follows is a brief description of these developments.

The classical definition of the ERR was introduced in the setting of a static mode I (opening mode) crack in a linearly elastic body. It was subsequently generalized to treat quasi-statically growing cracks and then dynamically growing cracks in either linear elasticity (infinitesimal strains) or finite elasticity. In the latter case, the theory was always developed using a (stress free) reference configuration, and in all cases singular crack tip stresses and strains were assumed leading to a finite, non-zero flow of (mechanical) energy into the crack tip. Consideration was also given to cohesive zone models which remove stress and strain singularities and for which the ERR is replaced by the rate of working of the cohesive zone stresses. However, for all of these theories, fracture surfaces were not modeled as dividing surfaces with excess physical properties.

The fracture theory being developed by the PIs endows the fracture surfaces with excess physical properties (momentum, internal energy, entropy, surface tension, etc) and incorporates a mutual body force correction to the differential momentum balance. These two modeling elements, the excess properties and the mutual force, together are intended to correct the bulk material constitutive behavior in a neighborhood of a fracture (dividing) surface for effects emanating from the long range intermolecular forces from the adjoining phases on either side of the fracture surface.

There have been a few previous attempts to develop fracture theories in which fracture surfaces are endowed with surface tension, internal energy, momentum and entropy, but none of them recognized the crucial role played by the jump momentum balance in deriving the “correct” fracture surface boundary conditions. In particular, these previous studies attempted to apply classical fracture surface boundary conditions along with the inclusion of fracture surface excess properties resulting in classical crack tip singular stresses and strains.

The new approach to modeling fracture studied under this AFOSR grant was introduced under the PIs previous AFOSR grant. The original effort considered a classical static Griffith crack problem in the context of the new theory utilizing fracture surface excess properties and a mutual force correction to the differential momentum balance. The problem was formulated and studied within both the deformed and reference configurations under the assumption that the linear Hooke’s law could be used to model the bulk material properties away from the fracture region. It also used a fracture boundary condition dictated by enforcing the jump momentum balance across the fracture surfaces. In the current AFOSR grant, the PI and his student T. Sendova began addressing the many theoretical questions left unanswered in the previous grant. First they addressed the question of showing a priori that the fracture boundary value problem resulting from the new theory must necessarily predict bounded crack tip stresses and strains and to determine which effect, the boundary condition derived from the jump momentum balance in the presence of crack surface excess properties or the mutual force correction to the differential momentum balance, is responsible for removing the crack tip stress and strain singularities seen in the classical fracture theories.

Against this backdrop, the principal accomplishments of this AFOSR project are summarized below.

- (I) The PI and T. Sendova proved various results associated with this canonical fracture boundary value problem that are contained in the paper (1).

- a. They showed that the use of Hooke's law in the deformed configuration was valid provided crack tip stresses and strains remain bounded and provided it is a valid approximation in a stress free reference configuration.
- b. They showed that ascribing constant surface tension to the fracture surfaces and using the appropriate crack surface boundary condition given by the jump momentum balance, leads to a sharp crack opening profile at the crack tip but predicts logarithmically singular crack tip stress.
- c. They also showed that a modified model with the surface excess properties being responsive to the curvature of the fracture surfaces, yields bounded stresses and a cusp-like opening profile at the crack tip.
- d. Further, they derived two possible fracture criteria in the context of the new theory. The first one is an energy based crack growth condition, while the second employs the finite crack tip stress the model predicts. The classical notion of energy release rate is based upon the singular solution, whereas for the modeling approach adopted here, a notion analogous to the energy release rate arises through a different mechanism associated to the rate of working of the surface excess properties at the crack tip.
- e. The theoretical results derived for the fracture modeling paradigm studied in (1) offer a number of potentially important benefits to practical fracture mechanics analyses. Besides the intriguing prospect of using a critical crack tip stress fracture criterion enabled by the finite crack tip stress field predicted by the model when one uses the jump momentum balance boundary condition on fracture surfaces along with a curvature dependent surface tension, there is no need in finite element calculations to employ singular elements at crack tips, cohesive zones or process zones, all of which entail difficulties to implement efficiently and accurately. With bounded crack tip stresses and strains resulting from use of the appropriate conditions, finite element implementation no longer needs to take account of singularities at crack-tips.
- f. The PI and his current Ph.D. student, Lauren Ferguson, are developing a finite element implementation of this new fracture theory. The chief challenge is implementing the jump momentum balance boundary conditions on fracture surfaces since when surface tension depends upon curvature, they involve third order tangential derivatives of the displacement. The theoretical results guarantee the required smoothness but the test function spaces are more complicated than classical fracture models. The main idea of the new numerical procedure is to view the crack surfaces and bulk body as separate material phases with their own constitutive behavior and numerical discretizations that are coupled through the jump momentum balance. This work will be in Lauren Ferguson's Ph.D. dissertation scheduled for completion in 2011.
- g. Subsequently T. Sendova and the PI have generalized the work in (1) to the more complicated setting of interfacial fracture. In (2) they show that one must now endow both the fracture surfaces and the bimaterial interface with excess properties in which surface energy has a dependence upon curvature. They then prove that as with the previous case of a crack within a single

phase material, the theory predicts bounded stresses and strains at the crack-tip and a cusp-shaped crack opening profile.

- (II) Simultaneously with this effort, the PI and his colleague Prof. K. R. Rajagopal initiated a new approach to fracture in the context of strain-limiting theories of elasticity. This program exploits a novel approach to modeling the mechanical response of elastic (that is non-dissipative) materials through implicit constitutive relations. The particular class of models studied can also be viewed as arising from an explicit theory in which the displacement gradient is specified to be a nonlinear function of stress. This modeling construct generalizes the classical Cauchy and Green theories of elasticity that are included as special cases. They had conjectured that special forms of these implicit theories that limit strains to physically realistic maximum levels even for arbitrarily large stresses would be ideal for modeling fracture by offering a modeling paradigm that avoids the crack-tip strain singularities characteristic of classical fracture theories. The simplest fracture setting in which to explore this conjecture is anti-plane shear. They demonstrated in (3) that for a specific choice of strain-limiting elasticity theory, crack-tip strains do indeed remain bounded. Moreover, the theory predicts a bounded stress field in the neighborhood of a crack-tip and a cusp-shaped opening displacement. The results confirm the conjecture that use of a strain limiting explicit theory in which the displacement gradient is given as a function of stress for modeling the bulk constitutive behavior obviates the necessity of introducing ad hoc modeling constructs such as crack-tip cohesive or process zones in order to correct the unphysical stress and strain singularities predicted by classical linear elastic fracture mechanics. In (3), they make a number of observations concerning implications of the new theory on fracture criteria.
- a. Since the theory presented above predicts stress and strain vanish at the crack-tip, the crack-tip is not a singular energy sink as in classical linear elastic fracture mechanics, and hence use of the classical local (to the crack-tip) fracture criterion based upon the Stress Intensity Factor or local Energy Release Rate is not available.
 - b. However, along any radial line extending from the crack-tip, the stress will quickly rise to a maximum and then decrease. That maximum will occur near to the crack-tip. This suggests a fracture criterion whereby the crack will extend whenever that near-tip maximum exceeds the fracture strength of the material.
 - c. As an alternative approach, one can develop a global fracture criterion, as described in (1) for example, that is readily implemented in numerical simulations. Moreover, one can also derive a local fracture criterion within the strain limiting theory employed here through introduction of crack-surface or crack-edge elasticity as exploited in (1). The key to utilizing the theory developed in (1) in the present context of strain limiting bulk constitutive theories is the demonstration above of bounded crack-tip stress and strain. Ultimately the choice of what fracture criterion to use in a particular application should be guided by experimental validation and ease of implementation.

THESES AND DISSERTATIONS

The first Ph.D. student support under this AFSOR project, Dr. Tsvetanka Sendova, wrote her Ph.D. dissertation on the theoretical developments described above. She graduated in August 2008 and subsequently took a two-year postdoctoral position at the Institute for Applied Mathematics and Its Applications at the University of Minnesota beginning in September 2008. The second graduate student support on this grant, Ms. Lauren Ferguson, worked on developing a finite element implementation strategy of the fracture approach based on viewing fracture surfaces as dividing surfaces with interval energy and surface stress. She is tracking to graduate by August 2011. The third graduate student supported during the final grant year is Mr. Mallikarjuna Muddamallappa who is beginning to develop a numerical code for implementing the second fracture modeling paradigm based upon the bulk strain limiting elastic constitutive relation. He is only a second year Ph. D. student and has several more years remaining in his Ph.D. studies. His dissertation will be devoted to continuing the development of the new fracture theory in the context of nonlinear, strain limiting elasticity.

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