Obtaining Fracture Properties By Virtual Testing And Molecular Dynamics Techniques

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ABSTRACT

Fracture critical parts of aerospace structures must have adequate life to withstand the cyclic load environment throughout their service usage. The safe-life analysis of these parts requires having comprehensive fracture mechanics data that are obtainable through the ASTM testing standards. These tests are costly and time consuming and in many cases can have impact on the program when needed data for life analysis are not available to designers. Any method that can be used to minimize testing can be of great help to the program. The proposed virtual testing technique can be extremely helpful to generate fracture toughness and fatigue crack growth data by using only the full stress-strain curve for the material under consideration. Results of fracture data generated by this method have been verified by test results for numerous aerospace alloys [1,2]. Excellent agreement between analysis and test data were obtained for both fracture toughness and fatigue crack growth rate allowable. However, it was realized that in some cases, the full stress-strain curve for the material does not exist in the literature and must be obtained through testing. For this reason and as an extension of this work, it is desirable to generate the full stress-strain curves by applying the multiscale modeling approaches [3] and therefore, making the above-mentioned virtual testing technique free from ASTM testing. Many multiscale modeling approaches have been recently used to predict the stress-strain response of a wide range of metals, including high strength, high toughness metals [3] and Nickel and Titanium-based super alloys [4], among others.

1 BACKGROUND

In general, multiscale modeling efforts rely on atomistic- or molecular-level information to predict the behavior of the material in response to applied loadings and environmental conditions. The effects of grain boundaries and dislocation are directly incorporated into the prediction of large-scale material behavior using an appropriately-chosen atomic potential. Because the prediction of stress-strain behavior of aerospace alloys from molecular-based multiscale approaches has not been rigorously pursued, current efforts are focused on developing models for these materials.

The application of the virtual testing methodology, together with the multiscale modeling and simulation technique for generating the full stress-strain curve, will be useful to the aerospace industry where the cost and time of testing can significantly be reduced.

Keywords: Virtual Testing, Fracture Allowables, Stress-Strain Curve, Molecular Dynamics, Multiscale Modeling

2 APPROACH

The Griffith theory of brittle fracture was established based on the available elastic energy, provided by the external load, to be release in order to extend the crack. All the consumed energy was depleted to create two new crack surfaces. Furthermore, it was shown that under the fixed grip case the amount of energy consumed to extend the crack (the energy release rate, $\partial Ue/\partial c$) is the same as the constant load condition. The Griffith theory was later extended by Farahmand [1] to account for ductile material where most of the available energy will be consumed for plastic deformation at the crack tip. The nature of plastic deformation is analogous to the uniform and non-uniform deformation for a uniaxial specimen where the area under the curve is the total energy necessary to fail the specimen. Therefore, this information will be useful to estimate the energy necessary to extend the crack in a plate. The nature of crack tip plastic deformation for aerospace metals, just like in the case of uniaxial tensile specimen, is of two kinds: The uniform plastic deformation near the crack tip, U_U, and non-uniform plastic deformation, U_F, at the crack tip. The total amount of energy associated with crack tip plastic deformation can be written as:

$$U_P = U_F + U_U \tag{1}$$

Therefore, the Griffith theory can be extended to account for the plastic deformation. It can be rewritten as:

$$\frac{\pi\sigma^2 c}{E} = 2T + \frac{\partial U_F}{\partial c} + \frac{\partial U_U}{\partial c} \tag{2}$$

where T is the surface tension of material. That is, the work done to break the atomic bonds and create two new crack surfaces. The derivation of the two terms associated with plastic deformation is shown in [1]. Equation (2) is the residual strength capability equation that describes a relationship between the crack length, 2c, and the fracture stress, σ. The second term in equation (2) is related to the energy necessary to plastically deform material by slip

mechanism through the energy under the stress-strain curve from necking up to the failure, W_F. The amount of deformation is designated by the h_F. Accordingly, the third term of equation (2) will be associated with crack tip plastic deformation by the consumed energy equivalent to the area under the stress-strain curve from yielding up to ultimate of the material.

$$\frac{\partial U_F}{\partial c} = W_F h_F \text{ and } \frac{\partial U_U}{\partial c} = W_U h_U \quad (3)$$

Therefore, the extended Griffith theory to account for the crack tip plastic deformation in terms of (3) is:

$$\frac{\pi\sigma^2 c}{E} = 2T + W_F h_F + W_U h_U \quad (4)$$

Equation (4) in its final format in terms of crack length, c, can be written as [1]:

$$2c = \frac{2E}{\pi\sigma^2\mu}\{2T + \bar{\sigma}_{UF}\varepsilon_{PN}h_F k + \frac{n}{n-1}\sigma_{TU}\varepsilon_{TU}[1-(\frac{\sigma_T}{\sigma_{TU}})^{n+1}]\, h_{min}[\frac{\varepsilon_{TF}\varepsilon_{TL}}{\varepsilon_{TU}\varepsilon_T}]^* [(\frac{\varepsilon_{TU}}{\varepsilon_{TL}})^{\frac{n-1}{n}} - 1]\beta\} \quad (5)$$

The quantities in equation (5) are obtainable from full stress-strain curve that can be obtained through uniaxial tensile test for material under consideration. The latter part of this work discusses the molecular dynamics approach to obtain the full stress-strain curve without conducting uniaxial tensile tests. Because equation (5) describes a relationship between the applied stress and critical crack length, 2c, the fracture toughness can be calculated via the stress intensity factor equation ($K=\beta\sigma\sqrt{\pi c}$). Figure 1 shows the calculated fracture toughness as a function of crack length for 2219-T6 aluminum alloy and was compared with test data extracted from [5]. Therefore, the extended Griffith theory can be used to generate material fracture toughness without conducting costly and time consuming tests which will be of great help to aerospace industry. This is referred to as virtual testing approach.

3 FATIGUE CRACK GROWTH

The virtual testing technique described above was extended to generate the fatigue crack growth data that is essential for life assessment of aerospace parts. The fracture toughness value obtained from equation (5) was used for the region III of the da/dN curve. The region I was estimated to be conservatively by ~ KIc/14 and the Paris Region through two fundamental assumptions [2], 1) the lower point in the Paris region of the fatigue curves has a

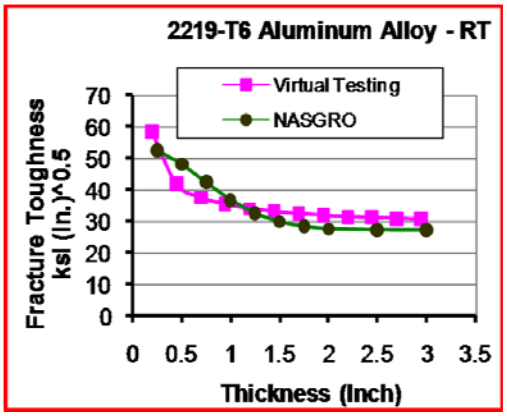

Figure 1: Comparison of estimated fracture toughness with test data [4].

material independent property (Figure 2) so that the ratio of the stress intensity factor at the lower point to the threshold value ($\Delta K/K_{th}$ for $R=0$) is ~ 1.125 for the crack growth rate per cycle, da/dN~1.0E-7 inch/cycle (~2.54E-6 mm/cycle). In the upper region of the da/dN curve (at the end of the Paris region), the ratio of the upper bound stress intensity factor and its critical value, K_c, ($\Delta K/K_c$ for R=0)

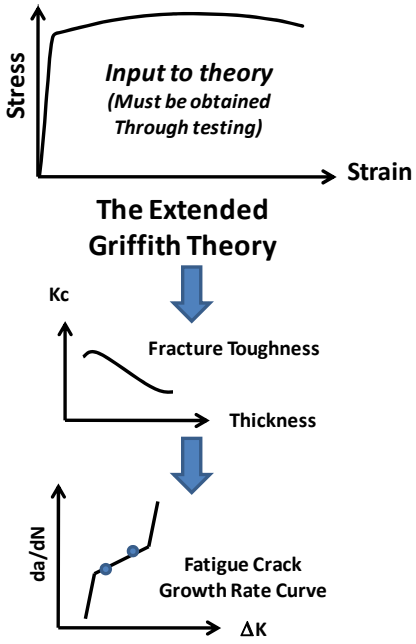

Figure 2: Using the extended Groffith theory to generate the da/dN curve [2].

is found to be ~0.9 for the da/dN ~0.005 inch/cycle (~0.127 mm/cycle). These two points are useful to plot the entire region II. The fatigue crack growth curve can then be

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plotted using the FNK equation (Forman, Newman, & de Koning) described in [5]. Figure 3 provides a comparison between the da/dN curve by the virtual testing technique and test data [5].

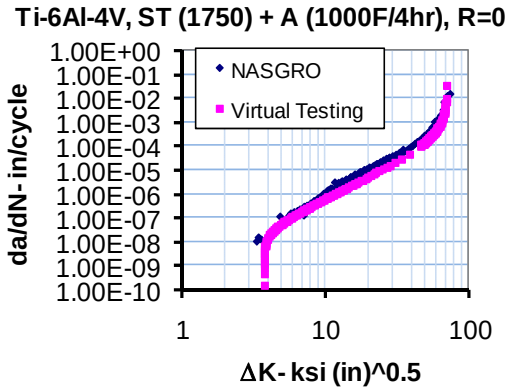

Figure 3: da/dN curve generated by the virtual testing and compared with the test data [5].

4 MOLECULAR DYNAMICS APPROACH

The above-described fracture and fatigue modeling approaches assume the presence of a material continuum. However, the prediction of the mechanical response of a metal at the atomic level requires molecular modeling in which a discrete atomic structure is modeled. Therefore, the fracture and fatigue laws cannot be directly coupled with molecular modeling unless the effective-continuum behavior of the atomic structure is established. In general, an effective continuum must meet two requirements in order to accurately predict the behavior of an atomic system:

1. Under identical applied far-field deformations (or loads), the atomic model and the effective continuum must have identical (or nearly identical) values of one or more scalar fields that are averaged over the atomic and effective continuum volumes. Examples of scalar fields include strain energy and individual components of the stress tensor.

2. The material points of the effective continuum volume must have the same kinematic motion as the atoms in the atomic model at the same locations.

Figure 4 shows an example of these points. The idealized 2D crystal structure of the metal has atomic coordinates that match the coordinates of the corresponding finite element nodes. For the same applied bulk deformation, the atom-node pairs must exhibit the same local motion. At the same time, the corresponding strain energy must be the same for the entire representative volume elements of the atomic and finite element models.

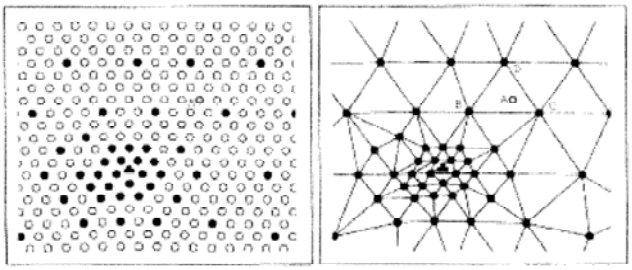

Figure 4: The location of atoms in a crystal on the left are the same as the locations of finite element nodes on the right, resulting in kinematic equivalence to the same applied bulk deformation (from Miller and Tadmor 2004).

A number of molecular dynamics (MD)-based approaches have been developed in the last decade to predict the constitutive response of metals and metal alloys by meeting one or both of these requirements. These methods have focused on predicting the mechanical response of metals on the atomic level based on applied macroscopic loads. These methods can be employed to generate stress-strain curves for metallic materials that can be used as an input into the above-described fracture and fatigue analyses.

The *Macroscopic, Atomistic, ab initio dynamics* (MAAD) modeling approach was developed [6] to simultaneously simulate tight binding, molecular dynamics, and finite element processes of a material element. In this scheme, the finite element mesh is fine enough such that the element sizes are on the order of the atomic spacing. The *Coarse-Grained Molecular Dynamics* (CGMD) approach was developed at about the same time [7]. The CGMD approach removes the tight-binding simulation component of the simultaneous simulation methodology such that only molecular dynamics and finite element simulations are used.

Perhaps the most well-known effective continuum approaches for crystalline materials is the *Quasi-Continuum approach* [8]. This approach takes advantage of the Cauchy-Born rule to establish an effective finite element domain that simulates the motion of the crystalline molecules. The effective properties of the finite element mesh is derived from an interatomic potential energy function, and an adaptive finite element technique is used to simulation the material response to large deformations. Higher-order elasticity theories have been used in

conjunction with the Quasi-Continuum method to model heterogeneous deformations.

The *Coupled Atomistics and Discrete Dislocation* (CADD) approach was developed [9] to incorporate dislocation plasticity into the molecular statics and effective continuum models. Therefore, dislocations generated within the atomics simulation region can effectively pass onto the continuum model region, such that the generation and behavior of dislocations can be modeled on separate length scales. Challenges for the CADD approach include the extension to dynamic problems and to three-dimensional simulations.

The *Bridging Domain Method* [10] couples molecular dynamics region with a continuum region that surrounds the molecular dynamics domain. A finite-sized overlap in the two models is called the bridging domain. The kinetic and potential energies associated with the bridging domains are a graded mixture of those associated with the molecular and continuum models. This approach can model the different time steps of the molecular and continuum models, and has been used in wave and crack propagation problems.

The *Bridging Scale* modeling approach [11] couples molecular dynamics simulations and continuum mechanics modeling by projecting the MD solution onto finite-element shape functions. As a result, the kinetic energies of the two simulations are decoupled and separate time step sizes can be used. Therefore, the finite element solution is not limited to the time scale of the molecular simulations.

The *Atomic-Scale Finite Element Method* (AFEM) was developed [12] to model crystalline materials and carbon nanotubes-based materials. This method directly incorporates atomic-potentials into the finite element method. A simple energy minimization is used to establish the mechanical behavior of the material. Although this approach has been used to analyze a wide range of nanotube-related problems, similar challenges remain as with the other methods discussed in this section. The application of these methods to problems of complex molecular structure with a wide-range of chemical bonding types and atomic varieties has yet to be achieved.

Yamakov et al. [13] used MD simulations to model the grain-boundary fracture behavior in Aluminum. Effective-continuum elastic properties and the effective-continuum decohesion law were established using energies associated with atomic forces near the crack tip.

5 SUMMARY

It is clear that the computational techniques are available to establish stress-strain curves for metals based on atomistic information. The future goals of this project are to establish stress-strain responses for a wide range of metal alloy systems that can be used as input into the fracture and fatigue models discussed herein to predict the bulk-level failure response without the need for experimental input. Results must be compared with test data to insure the validity of the computational technique.

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