

Crack Healing And Crack Closure Retardation Effect Through Release of Liquid Monomer In The Wake of Crack

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ABSTRACT

Designers are always looking for ways to reduce the weight and prolong the fatigue life of structural parts. This paper will discuss the benefit of self-healing materials. Self-healing materials possess the novel property of diagnosing any damage occurring to the structure, and repairing it autonomically like a living system. Various methodologies have been reported in the literature to impart self-healing properties in a synthetic materials system. One of the earliest and most successful methods for self healing deals with the release of liquid monomer in the wake of a propagating crack that eventually retards the crack growth [1]. The physics behind the crack retardation phenomenon in this situation has been variously attributed to the functionalization and eventual adhesion of the crack flanks due to curing polymer, and the crack closure effect due to the solidified polymer wedge behind the crack tip. Moreover, a competition between the time scales associated with healing chemistry occurs with the time scale associated with the cyclic loading in a fatigue loading environment. This competition determines the extent of crack retardation and its eventual arrest under fatigue loading scenario. Attention will be given to the crack arrest and its benefit to life extension of structural parts.

1 BACKGROUND

It is the goal of the aerospace industry to manufacture and design parts that can have an infinite fatigue life. One logical way of accomplishing this goal is to reduce the level of stress so that the possibility of a crack initiating and propagating will be remote and non-existent. However, by choosing this approach, there will be a significant weight penalty and costs associated with the program. Another approach to prolong the life of the structure is to select lightweight materials that have adequate strength, ductility and a high endurance limit value that could delay crack initiation when compared with traditional aluminum alloys. The problems with this method, unfortunately, are high costs associated with material availability and the complexity of manufacturing parts, which can be seen when comparing the application of aluminum alloys versus titanium.

The crack healing technique is another approach that can be implemented to retard and arrest the pre-existing crack in

the material in order to extend the fatigue life of the structural parts. This novel concept is based on retarding and ultimately healing the crack flanks due to curing polymer, and the crack closure effect due to the solidified polymer wedge behind the crack tip in the polymer. Towards this goal, a set of predictive modeling tools are developed that includes the physics of crack retardation along with the time scales associated with the healing chemistry and loading. These models will accurately predict the required choice of healing chemistry for a performance goal for self healing materials under a given service loading scenario [2]. The model will be discussed in the presentation. We have also undertaken an in depth parametric study to ascertain the effect of the thickness and the distance of the solidified polymer wedge from the crack tip, adhesion of the curing polymer with the crack flanks, time associated with healing, and various loading conditions on the healing efficiency of this class of materials. The results of this study will also be presented. Our modeling effort will finally arrive at a set of robust design protocols for efficient development of self healing materials.

Keywords: Crack healing, crack retardation, crack arrest, crack closure, monomer, multiscale modeling

2 APPROACH

The fatigue crack propagation and arrest in a self healing material being an extremely complex phenomenon. The choice of right healing chemistry for a given service loading environment is somewhat arbitrary. A number of costly and time consuming experimental iterations are required to arrive at the desirable self healing response for a material. An in depth knowledge of the physic-chemical phenomena occurring in this class of materials is thus required to accurately predict their healing efficiency. Because the crack healing process is effective at the presence of crack, the number of cycles to initiation (i.e. stage I) will remain the same and only the propagation phase will be affected by this phenomenon. White et al. [3] have developed a self-healing polymer that mimics many of the features of a biological system. Fig. 1 shows a three-stage healing process, accomplished by incorporating a microencapsulated healing agent (circular shape) and a catalytic chemical in an epoxy matrix. When crack is initiated in a high cycle fatigue environment, the presence of microencapsulated healing agent will be ruptured and disperse

the Dicyclopenta-diene (DCPD) monomer into the crack plane. The contact between the DCPD monomer and the catalyst (Grubbs) will initiate the polymerization and eventual healing process take place. That is, bonds between the two crack surfaces due to the presence of dispersed monomer and the catalyst (both embedded in the resin of composite material) can be established. Of course the process of crack healing (time to heal) is important because it defines the ability of two fractured surfaces to recover in the region just behind the crack tip.

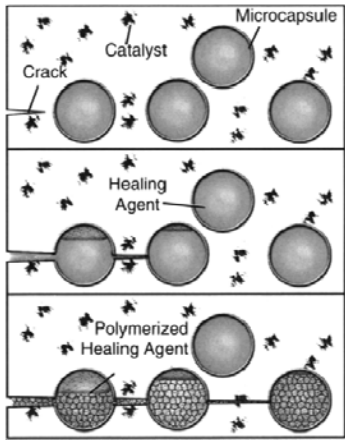


Figure 1: Three stages of crack healing process [3]

Figure 2 demonstrates the anticipated trend under the high cycle fatigue environment for a given polymer matrix with and without the presence of microencapsulated healing agent. Note that the S-N curve represents the total life of the part and therefore the crack healing process supposes to be effective only after the crack initiation stage. In Figure 2, three curves are plotted which represent the S-N trend for the material without the healing process and the other two for fully and partially effective scenario. That is, the released monomer at the mouth of the crack will rapidly interact with the catalyst and close the crack flanks effectively. On the other hand if the healing chemistry for establishing bonds at the crack wedge is time consuming, the only benefit which this process will have is to leave monomer particles at the wake of the crack and cause retardation. This ineffectiveness will be also true for the situation that cracking will take place rapidly due to either material lack of ductility or high load magnitude. It is logical to say that this process is also stress ratio dependent. The healing chemistry will be more effective for stress ratio $R=-1$, where the mean stress is zero and crack flanks will close at each cycle. At higher stress ratio, $R \geq 0$, the two crack mouths will not close and the process of healing is not effective. Figure 3 demonstrates the effectiveness of the healing process with respect to stress ratio. Note that in the case of $R=-1$, the curve is shifted upward due to healing process to indicated that the healing mechanism is most effective when crack mouths are in contact with each other.

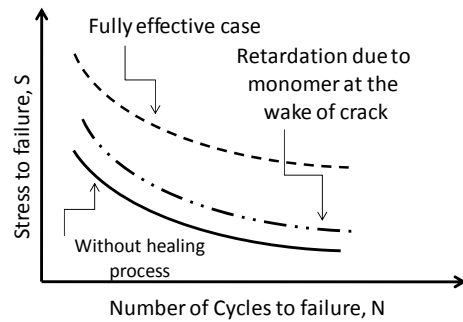


Figure 2: To illustrate the effectiveness of the crack healing process.

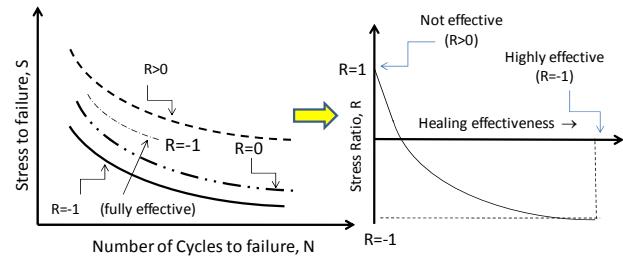


Figure 3: Effect of crack healing as a function of stress ratio, R . For $R \geq 0$ the healing process may not be effective

Material with low fracture toughness or parts under high load cycle magnitude cannot benefit from self healing process. Under high load magnitude where crack is advancing rapidly, the healing mechanism cannot be effective to close the crack flanks. This scenario can be also true for the case of material with low fracture toughness. That is, material with low K_{Ic} , where fast fracture can occur, polymerized healing agent cannot be effective because of inadequate time to form a wedge at the crack tip. However, the crack arrest or fail safe feature embedded in

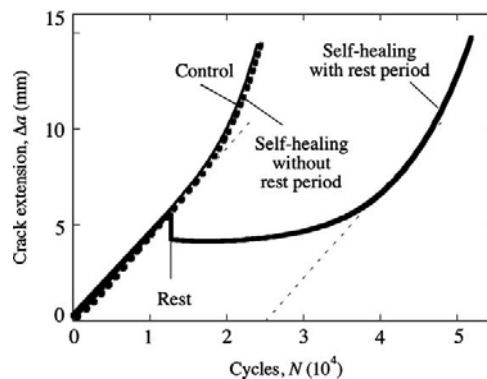


Figure 4: When crack is near stage III or lack of material ductility, crack healing process cannot be effective [3].

design of parts are helpful for the healing mechanism to occur in the present of material with low K_{Ic} value. Figure 4 is taken from reference [3] where two cases with and without self healing process is demonstrated. In this figure,

without applying self healing process, or when crack is near stage III crack growth rate, the healing time is inadequate for polymerization at the crack surfaces to take place.

3 COMPUTATIONAL MODEL

Successful computational models that can predict the self healing response of a material should incorporate the physics involved at different length and times scales during the healing of the material. Fatigue type of loading possesses an inherent time scale while the polymerization of monomers to a solid wedge is dictated by the time scale associated with healing of that particular monomer. The presence of that polymer wedge (Figure 5) in the wake of the crack tip along with the adhesion effect between the crack flanks and the functionalized wedge at the nanoscale give rise to the macroscopic crack retardation behavior. The physical situation is explained in Figure 6: Effective stress intensity factor range ΔK_{eff} that is responsible for driving a fatigue crack gets substantially reduced due to the presence of these two effects. Consequently, ΔK_{eff} at the crack tip

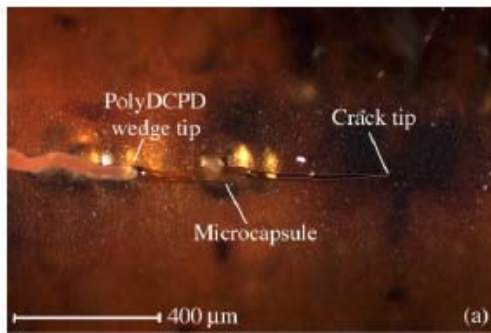


Figure 5: Evidence of the presence of a polymerized wedge in the wake of a crack in a self-healing material [4].

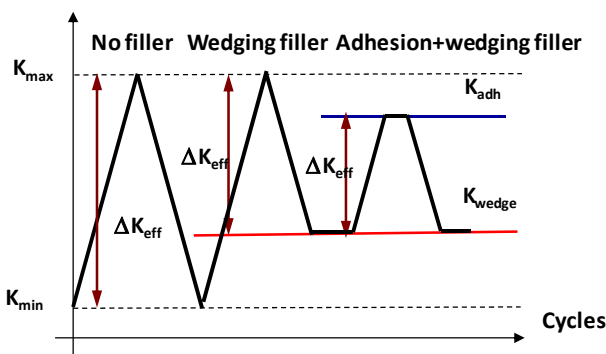


Figure 6: Reduction of effective stress intensity factor range (ΔK_{eff}) due to wedging and adhesion effect.

reduces substantially so that rate of crack propagation is also diminished. The computational model developed by us depends on a cohesive description of fatigue crack propagation [6]. Note that, the model should incorporate the irreversibility arising from damage accumulated ahead

of the fatigue crack tip during cyclic loading process. This property enables the model to propagate subcritical crack growth. To wit, rate of change of cohesive stiffness is expressed as:

$$\dot{k}_c = -\frac{1}{\alpha} N_f^{-\beta} k_c \dot{\Delta}_n \quad \text{if } \dot{\Delta}_n \geq 0, = 0 \quad \text{otherwise}$$

where, $\dot{\Delta}_n$ is the rate of change of normal separation, N_f is the cycles to failure, α and β are the parameters of the Paris curve, respectively. Wedge effect has been incorporated to this model through a novel contact enforcement model, while the adhesion effect is taken through a standard cohesive model with reversed thermodynamics. The resulting cohesive law with wedging effect is depicted in Figure 7. Prout-Tompkins phenomenological model of the

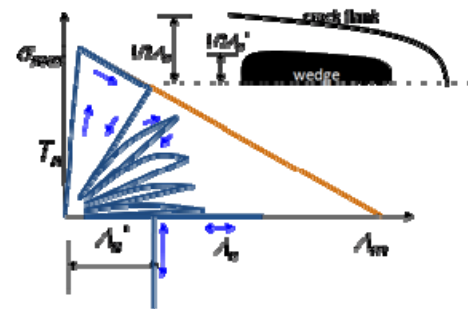


Figure 7: Schematic of the cohesive model with crack closure effect.

cure kinetics relation is [7]

$$\frac{d\alpha}{dt} = B(T)(1-\alpha)^n \alpha^m$$

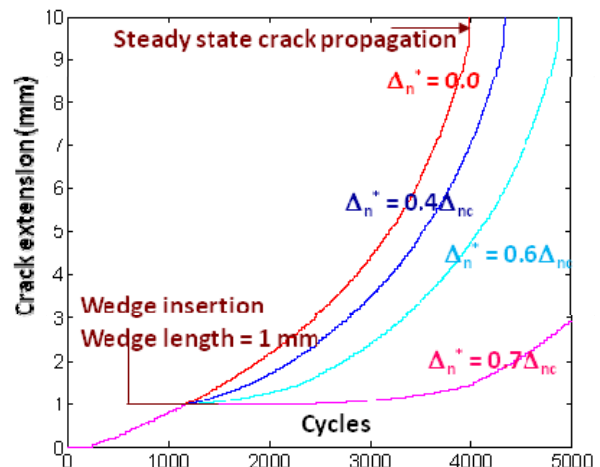


Figure 8: Effect of wedge thickness on crack

where α denotes the degree of cure that evolves between 0 retardation (uncured state) and 1 (fully cured state), $d\alpha/dt$ is the rate of reaction, $B(T)$ is a temperature-dependent rate

constant generally described by an Arrhenius equation, n and m are the fitting parameters. Our simulations have resulted in values of 0.05 and 2.0, respectively for the fitting parameters. Healing kinetics and resultant evolution of stiffness of the polymeric wedge have been found through a coarse-grained Monte Carlo simulation process that can take into account the molecular level mechanisms responsible for this evolution of materials properties. Stiffness of the polymerizing wedge can be related to its thickness through the equations described in [2]. Time scale associated with the healing process can be written as $\tau_{\text{heal}}=1/B$, and that related to the crack propagation is

$$\tau_{\text{crack}} = \frac{l_c}{da/dN\omega},$$

with l_c as the cohesive zone length, and ω as the frequency of the applied loading.

4 RESULTS AND DISCUSSION

Self-healing performance depends on a large number of parameters. The model described in the last section is capable to incorporate a number of these models, and predict the effect of variation of individual parameters on the crack retardation and eventual arrest. In the following, we present the effect of a few selected microscopic parameters on the macroscopic rate of crack propagation in self healing materials. Figure 8 shows the effect of thickness of the inserted wedge Δ_n^* expressed as a percentage of the critical crack opening displacement Δ_{nc} .

All the wedges have been inserted when the crack extension reaches 1 mm while the length of the wedge has been kept constant at 1 mm. Note from this figure that, as the wedge thickness increases, the crack propagation rate reduces drastically. So, our model can predict the experimental observation that thickness of the polymerized wedge at the wake of the crack can control the crack growth rate. Moreover, the model predicts that the effect of thin wedges is quite minimal on the rate of crack propagation. To reduce the crack extension substantially, one needs to insert a wedge of thickness at least half of the critical crack opening displacement. Figure 9 shows the effect of distance of the polymeric wedge from the crack tip. All the wedges have a length of 5 mm, and are introduced when the fatigue crack extends by 2 mm. It can be clearly seen that the wedge that extends up to the crack tip is the most effective in retarding crack growth; wedges inserted just 2 mm behind the crack tip has a minimal effect on the overall crack propagation. This set of simulations clearly points out that the modification of crack closure due to wedging effect diminishes very quickly as the distance between them increases. The wedge cannot shield the crack tip effectively (as depicted in Figure 6) in this scenario. We have also

considered the effect of the length of the wedges inserted at the crack tip on crack retardation. The inset shows the crack extension against the loading cycles for wedges with lengths 1, 2 and 5 mm respectively. Note that, the length of the wedge does not have any effect on the crack propagation as long as only wedging effect is considered. In conclusion, it can be said that, the proximity of the wedge from the crack tip rather than its extent is more important for successful crack retardation in self-healing polymers.

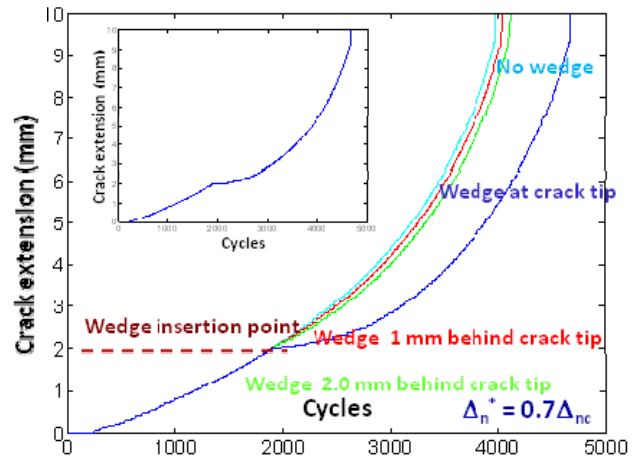


Figure 9: Effect of wedge length and proximity to the moving crack tip on crack retardation [6].

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