A MULTISCALE MODEL FOR THE PREDICTION OF FATIGUE CRACK GROWTH BEHAVIORS OF POLYMER NANOCOMPOSITES

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ABSTRACT

In this study, we develop the methodology to predict the fatigue crack growth of the thermoset polymer nanocomposites, based on multiscale approach. The experimentally observed microscopic energy dissipating mechanisms (nanoparticulate debonding, the subsequent plastic yield of nanovoids, and localized shear banding) are reflected in the proposed methodology. The predicted results show satisfactory agreements with respect to experimental data. The achievement of this study is expected to elucidate the complex phenomenon of fatigue crack growth as well as provide high efficiency with satisfactory predictions.

1 INTRODUCTION

It is a well-known fact that the embedded nanoparticles enhance the stiffness, yield strength, fracture toughness, and fatigue crack growth behaviors of polymer nanocomposites. For the material design of polymer nanocomposites, the multiscale models to predict the mechanical properties (stiffness [1, 2], yield strength, and fracture toughness) and mechanical behaviors have been developed. Even though it is important to predict fatigue crack growth of polymer nanocomposites, it has not been treated for the fatigue crack growth of polymer nanocomposites. Recently, Kothmann *et al*. [3] reported that the fatigue crack resistance of polymer nanocomposites is critically related to the following microscopic damaging mechanisms: "nanoparticulate debonding and the subsequent plastic yield of nanovoids", "localized shear banding". In this study, the multiscale model to predict fatigue crack growth of polymer nanocomposites is proposed, which is validated by comparison with the experimental data.

2 THE PROPOSED MULTISCALE MODEL

The strain energy release rate of polymer nanocomposites can be described as follows:

$$G_{\mathrm{I}}^{\mathrm{comp}} = G_{\mathrm{I}}^{\mathrm{mat}} + \sum_i \Delta G_i \tag{1}$$

Here, the microscopic energy dissipation can be quantified by J-integral as follows:

$$\Delta G_i = 2 \times \int_0^{\rho^*(\phi=\pi/2)} u_i \, d\rho \tag{2}$$

The detail formulations on the microscopic energy dissipation can be found in Refs. 4-6. From the relation between the strain energy release rate and stress intensity factor, the stress intensity factor of polymer nanocomposites can be defined as follows:

$$K_{\mathrm{I}}^{\mathrm{comp}} = K_{\mathrm{I}}^{\mathrm{mat}} \times \zeta \tag{3}$$

where ζ can be obtained by the following form:

$$\zeta = \sqrt{\frac{1}{1-f_{\mathrm{p}}\left(\psi_{\mathrm{db}}+\psi_{\mathrm{py}}+\psi_{\mathrm{sb}}\right)} \times \frac{E_{\mathrm{comp}}}{1-\nu_{\mathrm{comp}}^{2}} \times \frac{1-\nu_{\mathrm{mat}}^{2}}{E_{\mathrm{mat}}}} \tag{4}$$

where f_{p} is volume fraction of nanoparticle and ψ_{db}, ψ_{py}, and ψ_{sb} are the contribution of each microscopic energy dissipating mechanisms [4-6].

Fatigue crack growth of polymer matrix and polymer nanocomposites can be described by the following forms:

$$\begin{cases} \dfrac{da_{\mathrm{mat}}}{dN} = f_{\mathrm{mat}}\left(\Delta K_{\mathrm{I}}^{\mathrm{mat}}\right) \\ \dfrac{da_{\mathrm{comp}}}{dN} = f_{\mathrm{comp}}\left(\Delta K_{\mathrm{I}}^{\mathrm{comp}}\right) \end{cases} \tag{5}$$

Here, the stress intensity factors of polymer nanocomposites can be described as follows:

$$\left(K_{\mathrm{I,max}}^{\mathrm{comp}}, K_{\mathrm{I,min}}^{\mathrm{comp}}, \Delta K_{\mathrm{I}}^{\mathrm{comp}}\right) = \left(K_{\mathrm{I,max}}^{\mathrm{mat}}, K_{\mathrm{I,min}}^{\mathrm{mat}}, \Delta K_{\mathrm{I}}^{\mathrm{mat}}\right) \times \zeta \tag{6}$$

Then, the relationship of fatigue crack growth behaviors between polymer matrix and polymer nanocomposites can be described as follows [7]:

$$f_{\mathrm{comp}}^{-1} = f_{\mathrm{mat}}^{-1} \times \zeta \tag{7}$$

Using this relationship, the Paris Law of polymer nanocomposites can be determined as follows:

$$\frac{da}{dN} = C_{\mathrm{mat}} \times \left(\Delta K_{\mathrm{I}}^{\mathrm{mat}}\right)^{m_{\mathrm{mat}}} = C_{\mathrm{mat}} \times \left(\frac{1}{\zeta} \times \Delta K_{\mathrm{I}}^{\mathrm{comp}}\right)^{m_{\mathrm{mat}}} = C_{\mathrm{comp}} \times \left(\Delta K_{\mathrm{I}}^{\mathrm{comp}}\right)^{m_{\mathrm{comp}}} \tag{8}$$

Here, the Paris coefficients can be determined by the following form:

$$\begin{cases} C_{\mathrm{comp}} = C_{\mathrm{mat}} \times \zeta^{-m_{\mathrm{mat}}} \\ m_{\mathrm{comp}} = m_{\mathrm{mat}} \end{cases} \tag{9}$$

3 MODEL VALIDATION

We predict the fatigue crack growth behaviors of polymer nanocomposites to validate the proposed multiscale model. Epoxy/SiO_2 nanocomposites (average diameter: 20nm) are employed, and sinusoidal load ($K_{\mathrm{I,min}}/K_{\mathrm{I,max}}$=0.1) is assumed. System detail can be found in Ref. 3.

The fatigue crack propagation behaviors of the epoxy/silica nanocomposites are predicted and listed in Table 1. For the various weight fraction systems, the ranges of stress intensity factors ($\Delta K_{\mathrm{I}}^{\mathrm{comp}}$) for the fatigue crack growth rate (da/dN) are predicted by using Eq. (7). To validate the proposed approach, the experimental data [3] are compared with the predicted fatigue crack growth behaviors for 5wt% system. Even though the predicted results are slightly higher than the experimental data, the results show satisfactory predictions by allowing for the uncertainties in the manufacture of polymer nanocomposite systems (e.g., imperfections in the polymer domain, locally agglomeration of nanoparticles, and variation in the nanoparticulate diameters), and the measurements of the fatigue crack propagation behaviors. When we consider the amplitude of error bar of critical stress intensity factor is about 0.04 MPa·$m^{1/2}$ for the 5wt% nanocomposite system, the prediction seems to be in well agreement with the corresponding experimental results [3]. Especially, it is noteworthy that the proposed approach is applicable in every fatigue crack propagation regimes.

To validate the current model, the further comparison with experimental data set is conducted, whose results are listed in Table 2. The predictions show considerably good agreement with another experimental data set [1]. These experimental systems are also composed of epoxy and rigid spherical silica nanoparticles, whose average diameters are 20nm. The epoxy elastic modulus and the critical stress intensity factor of neat epoxy are determined by Table 1 of Ref. 8 in revision as 2.96 GPa and

0.51 MPa·m$^{1/2}$, respectively. The other input mechanical properties are listed in Table 1 of Ref. 7. The reference data of Table 2 are obtained from the Fig. 3 of Ref. 8.

It is worth mentioning that the major contribution of this study is that the master curves for thermoset polymeric nanocomposites can be predicted for various weight fractions of nanoparticles if the fatigue crack growth behavior of the neat thermoset polymer matrix is predetermined. In Table 1, we employed the experimental data of fatigue crack growth behavior of neat epoxy matrix as base curves for the generation of master curves. For neat epoxy matrix, any predetermined fatigue crack growth curve of epoxy/silica nanocomposites, including an arbitrary weight fraction of nanoparticles, can also be employed as the base curve.

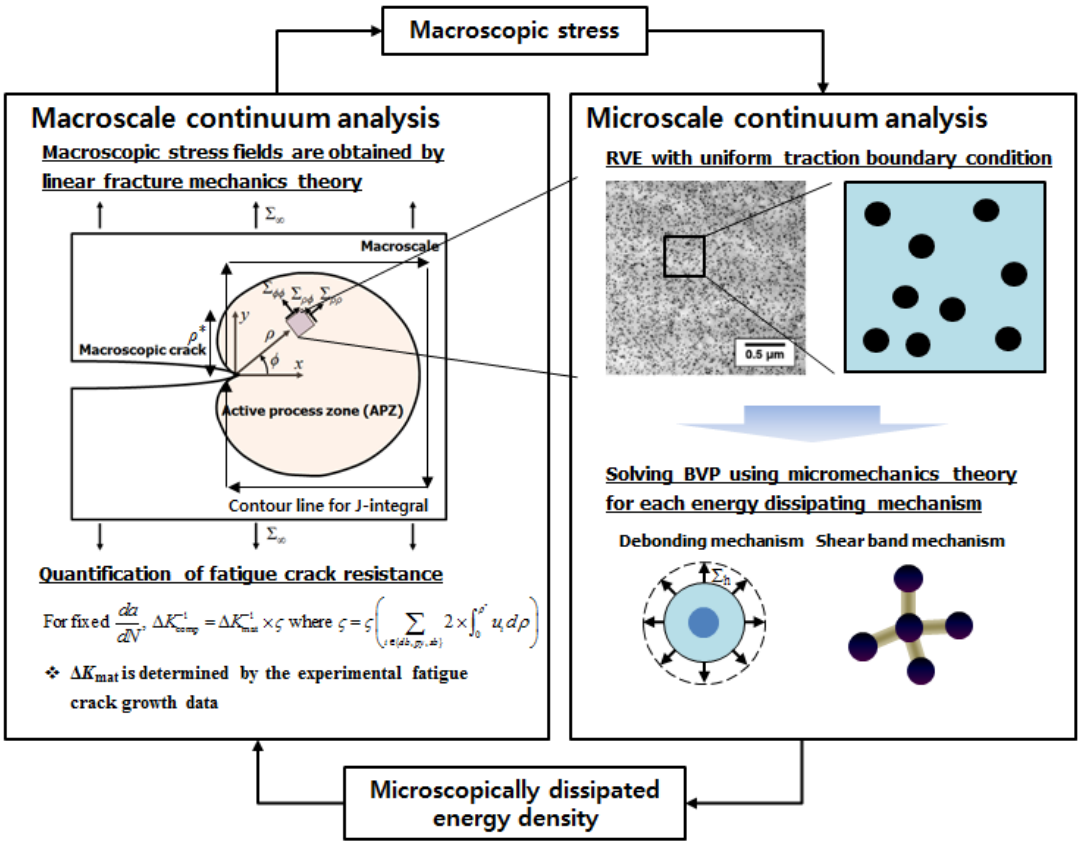

Figure 1. The proposed multiscale framework to predict fatigue crack propagation behaviors of the thermoset polymer nanocomposites by considering the microscopic energy dissipating mechanisms [7]

Table 1. Influence of weight fraction on the fatigue crack growth of nanocomposites [7] and validation by comparison with experimental reference data [3]

$\log_{10}(da/dN)$	Range of stress intensity factors (MPa·$m^{1/2}$)							Stages of crack growth
	0wt%	1wt%	2wt%	3wt%	4wt%	5wt%	5wt% (experiments)	
-5.502	0.269	0.280	0.293	0.308	0.325	0.347	0.314	Threshold regime
-5.360	0.271	0.283	0.296	0.311	0.329	0.350	0.324	
-5.219	0.275	0.286	0.299	0.315	0.333	0.355	0.334	
-5.077	0.280	0.291	0.305	0.320	0.339	0.361	0.344	
-4.935	0.286	0.298	0.312	0.328	0.347	0.369	0.355	
-4.794	0.295	0.307	0.321	0.337	0.357	0.380	0.367	
-4.652	0.305	0.317	0.332	0.349	0.369	0.393	0.379	
-4.510	0.316	0.329	0.345	0.362	0.383	0.408	0.392	Stable regime (Paris regime)
-4.369	0.330	0.343	0.359	0.377	0.399	0.425	0.405	
-4.227	0.344	0.358	0.374	0.393	0.416	0.444	0.418	
-4.085	0.358	0.373	0.390	0.410	0.434	0.462	0.432	
-3.944	0.372	0.388	0.405	0.426	0.451	0.480	0.446	
-3.802	0.385	0.401	0.420	0.441	0.467	0.497	0.460	
-3.660	0.397	0.414	0.433	0.455	0.481	0.513	0.474	
-3.519	0.408	0.425	0.444	0.467	0.494	0.526	0.488	
-3.377	0.417	0.434	0.454	0.477	0.505	0.538	0.501	
-3.235	0.424	0.442	0.462	0.486	0.514	0.547	0.514	
-3.094	0.430	0.448	0.469	0.492	0.521	0.555	0.525	
-2.952	0.435	0.453	0.474	0.498	0.527	0.561	0.535	
-2.810	0.439	0.457	0.478	0.502	0.531	0.566	0.544	Unstable regime
-2.669	0.442	0.460	0.481	0.506	0.535	0.570	0.551	
-2.527	0.444	0.463	0.484	0.509	0.538	0.573	0.557	
-2.385	0.446	0.465	0.486	0.511	0.540	0.576	0.562	
-2.244	0.448	0.466	0.487	0.512	0.542	0.578	0.565	
-2.102	0.449	0.467	0.489	0.514	0.543	0.579	0.568	

※ In the experimental reference paper [3], it was reported that the 0.04 MPa·$m^{1/2}$ of amplitude of the error bar is involved in the prediction of critical stress intensity factor for 5wt% nanocomposite system. It can be expected that the error in the prediction of range of stress intensity factor would be similar values.

Table 2. Further comparison with another experimental data set [8] to validate the current predictive model [7]

Properties [MPa·m$^{1/2}$]	Matrix	Composites			
		4wt%		7.8wt%	
		Current model	Experimental data	Current model	Experimental data
ΔK_{th}	0.11	0.14	0.15-0.17	0.19	0.18-0.19
K_{Ic}	0.51	0.62	0.60-0.70	0.85	0.75-0.85

4 CONCLUSIONS

In this study, a novel attempt to predict fatigue crack propagation behaviors of the thermoset polymer nanocomposites has been explored. At low weight fraction systems, the predictions showed a highly satisfactory agreement with the corresponding experimental data. We believe that the proposed multiscale model can serve as a guideline for characterizing master curves of fatigue crack growth behavior for various weight fraction systems. The model can also help in developing material designs of thermoset polymer nanocomposites to achieve high fatigue crack resistance by using the microscopic energy dissipating mechanisms.

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