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Multiscale analysis on the toughening behavior of thermoplastic modified epoxy

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ABSTRACT

Epoxy resins are widely used as phase materials of matrix in fiber-reinforced composites. To overcome brittleness of cross-linked epoxy, thermoplastic modified epoxy has been extensively studied. However, specific toughening mechanism of thermoplastic modified epoxy has not been established in molecular viewpoint. Allegedly, toughening mechanisms – particle debonding, plastic yielding of nanovoids, and localized shear banding – are primary origin of fracture toughness enhancement. The purpose of this study is to investigate the contribution of each toughening mechanism. In this study, PES is used as a toughening agent for the cross-linked epoxy composed of TGAP and DDS. Cohesive interface is also considered as it can affect toughening mechanisms.

As a result, methodology of construction of finite element PES/epoxy model with cohesive interface is proposed. Observation of stress distribution of the model and toughening mechanisms expected to enhance fracture toughness will be studied later.

1. INTRODUCTION

Cross-linked epoxy has usually been composed of CNT, graphene or nanofiller to make various nanocomposites because of following strong points – high adhesiveness, high stiffness, creep resistance, and thermal resistance. But cross-linked epoxy system has weak toughness due to its brittleness. Therefore, enhancing the fracture toughness of epoxy system is critical issue. To enhance fracture toughness, epoxy is often modified by adding toughening agents like rubber, thermoplastic, and silica particle.

M. Quaresimin *et al*. analyzed three main toughening mechanisms – particle debonding, plastic yielding of particles, and localized shear banding –. They showed that energy dissipation occurs because of these mechanisms and it results in enhancement of fracture toughness by analyzing 12 cases of different nanocomposites.

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To investigate the contribution of each toughening mechanism, proper analysis model must be proposed.

In this study, the multiscale modeling strategy is proposed by combining MD simulation with finite element model. Different from micromechanics based model, it can reflect various particulate sizes and interfacial treatment by changing operators of nanostructure in MD simulation. Interfacial debonding mechanism is reflected in the cohesive interface zone model. Cohesive parameters are determined by traction-separation model obtained from MD simulation.

2. Cohesive zone modeling through MD simulation

In this study, cohesive zone is applied to describe interfaces between particles and matrix to more precisely. In order to discuss influence of cohesive interfaces on particle debonding, normal traction-separation model between polyether sulphone (PES) particle and epoxy is obtained. Result of shear traction-separation has not been obtained yet. In this study, shear traction-separation model is assumed to have half critical stress and doubled failure displacement.

The employed epoxy is fully cross-linked, and cross-linking simulation is conducted by close contact method. Both PES and epoxy are assumed to be elastoplastic model with linear hardening. The plastic parameters are given in Table 1.

Table 1. Elastoplastic properties of PES and epoxy

	Yield stress (GPa)	Hardening modulus (GPa)
PES	0.1418	0.03636
Epoxy	0.2446	0.1494

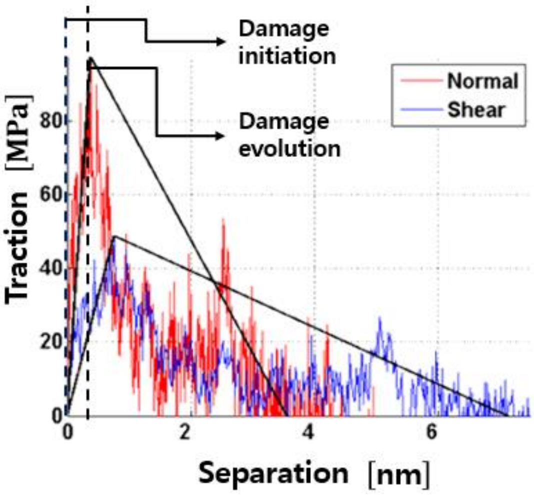

Fig. 1. Traction-separation model of PES/epoxy composites obtained from MD simulation

The cohesive parameters are obtained from above linear fitting result. Table 2. Shows the cohesive parameters of PES/epoxy composites conducted on this study.

Table 2. Cohesive parameters of PES/epoxy composites

	T-S elastic stiffness (GPa/μm)	Maximum nominal stress (GPa)	Displacement at failure (μm)
Normal	256.8	0.0976	0.003558
Shear	64.2	0.0488	0.003558

3. Finite element analysis of toughened epoxy

Construction of model of toughening mechanisms is necessary, as the contribution of each toughening mechanism can be evidently investigated by observing the model. In order to realize toughening mechanisms of toughened epoxy, RVE needs to be modeled and analyzed by finite element method with former cohesive parameters. The sequence of analysis in this study is shown in Fig. 2.

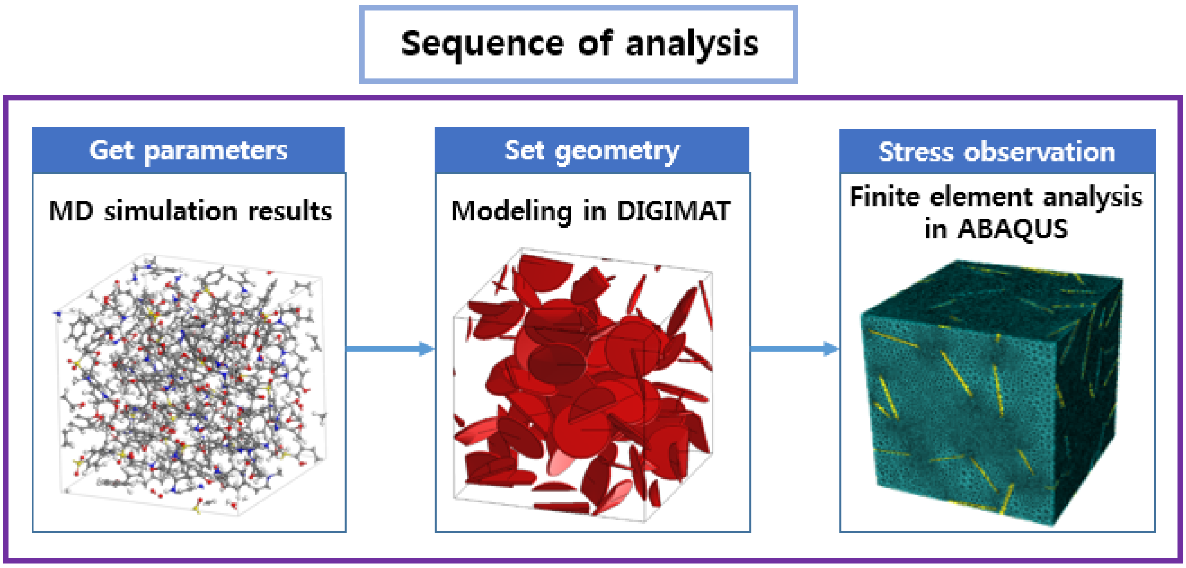

Fig. 2. Sequence of finite element analysis of toughened epoxy

In previous section, elastoplastic properties and cohesive parameters are deduced from MD simulation. RVE can be modeled in DIGIMAT with given particle volume fraction and aspect ratio. Finite element mesh can also be generated by ABAQUS. Given macroscopic strain, microscopic displacement field is able to be obtained by using ABAQUS.

4. Conclusion

In this study, multiscale analysis strategy considering MD simulation is proposed. Particle debonding regions are modeled by applying cohesiveness to interface of PES/epoxy model. But the way how to construct distinguished portions of shear banding and plastic yielding of nanovoids on the RVE model is not established yet.

In the future work, construction of adjusted model which can consider all three toughening mechanisms will be studied later. Observation of stress distribution of the model and toughening mechanisms expected to enhance fracture toughness will also be studied later.

In addition, analytic formulation of each toughening mechanism will be progressed. [M. Zappalorto et al.]

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