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Prediction of viscoelastic behaviour of nanoparticle-reinforced polymer composites by multiscale analysis

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A multiscale material modelling has grown to become a major scientific domain for the reliable prediction of various types of nanocomposites [1]. In this study, we present a multiscale modeling framework that relies on the molecular dynamics (MD) simulation and micromechanics to predict the viscoelastic behavior of nanoparticle-filled polymer composites [2]. In order to bridge the gaps between the nano and microscale properties of the nanocomposites, the micromechanical viscoelastic model considering nanoparticle size, interface properties, and strain-rate effect is newly derived using the concept of the ensemble-volume averaged method [3,4]. The physical properties at interfacial region between the matrix and nano-inhomogeneities are estimated by MD simulations, and the determined parameters are applied to the micromechanical model [4]. Based on the proposed method, a series of numerical simulations of the composites are conducted to elucidate the potential of the present model [2].

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REFERENCES

[1] J. LLorca, C. González, J.M. Molina-Aldareguía, J. Segurado, R. Seltzer, F. Sket, M. Rodríguez, S. Sádaba, R. Muñoz, L. P. Canal, Multiscale modeling of composite materials: a roadmap towards virtual testing. *Adv. Mater*., Vol. **23**, pp. 5130-5147, 2011.

[2] B.J. Yang, H. Shin, H. Kim, H.K. Lee, Multiscale analysis of strain rate and adhesive energy dependent viscoplastic damage model for nanoparticulate composites. in preparation.

[3] B.R. Kim, S.H. Pyo, G. Lemaire, H.K. Lee, Multiscale approach to predict the effective elastic behavior of nanoparticle-reinforced polymer composites. *Interaction and Multiscale Mech*., Vol. **4**, pp. 173-195, 2011.

[4] B.J. Yang, H. Shin, H. Kim, H.K. Lee, A combined molecular dynamics/ micromechanics/finite element approach for multiscale constitutive modelling of nanocomposites with interface effects. *Appl. Phys. Lett*., Vol. 103, pp. 241903, 2013.