Editorial corner – a personal view

Challenges in fracture toughness modelling of nanocomposites

B. Lauke^{1}, J. Karger-Kocsis²*

¹Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, D-01069 Dresden, Germany

²Department of Polymer Engineering, Faculty of Mechanical Engineering, Budapest University of Technology and Economics, MTA-BME Research Group for Composite Science and Technology, Műgyetem rkp. 3, H-1111 Budapest, Hungary

A basic question when modelling the fracture toughness of hybrid polymer composites is whether or not the particles' agglomerations are considered. Note that even in microparticle reinforced polymers the distribution of the particles is locally inhomogeneous because they get into contact as a consequence of production. In nanoparticle filled elastomers particles agglomerate and the agglomerates build even larger structures. Consequently, if we consider the close neighbourhood of a single particle there exists a much higher particle density than in larger distances. Such behaviour can be described for example by pair distribution functions (DOI: [10.1016/j.compositesb.2014.01.002](https://doi.org/10.1016/j.compositesb.2014.01.002)). Close particles cause high stress or strain concentrations in the matrix in between. This fact must be considered in strength and fracture toughness modelling. Filled polymer composites have been studied extensively because of their technological and scientific importance (DOI: [10.1007/BF01160743](https://doi.org/10.1007/BF01160743); DOI: [10.016/j.compositesb.2008.01.002](https://doi.org/10.016/j.compositesb.2008.01.002); DOI: [10.1016/0266-3538\(88\)90009-7](https://doi.org/10.1016/0266-3538(88)90009-7)). Generally, crack tip blunting, crack pinning, localized shear bands, debonding of particles as plastic voiding and localized plastic shear yielding were found to be responsible for the increase of toughness in thermoset composites. Models that consider such effects are able to describe some of the experimental results properly (DOI: [10.1007/s10853-009-4064-9](https://doi.org/10.1007/s10853-009-4064-9); DOI: [10.1016/j.compotech.2009.12.024](https://doi.org/10.1016/j.compotech.2009.12.024)). Also the effect of particle size on plastic void growth has been taken in account (DOI: [10.1016/j.mechrescom.2015.2.002](https://doi.org/10.1016/j.mechrescom.2015.2.002)). Homogeneous particle

distribution cannot be expected in 'real' materials. Increased number of nearest neighbours in microparticle filled composites and agglomerate formation in nanocomposites must be considered. Stiffness is not influenced by these events because at small deformations no debonding occurs. However, if strength or fracture toughness are computed, such local heterogeneities should be considered. As basic mathematical and experimental data are available, the modelling should involve this structural level. In the first step any mathematical pair distribution function can be used to calculate the number of particles close to the chosen one in the ensemble. High stress concentration in between such a pair may initiate debonding. The ligament in between the debonded particles becomes unloaded and their outer region overloaded accompanied with yielding. Debonding does not contribute much to energy dissipation but triggers matrix yielding that enhances the toughness. Debonding of particles leads to a reduction of tensile strength, too. Let us go in this direction to get a deeper understanding in the mechanical and fracture mechanical behaviours!

Dr. Bernd Lauke

Prof. Dr. Dr. h.c.
József Karger-Kocsis
Editor-in-Chief

*Corresponding author, e-mail: laukeb@ipfdd.de
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