



On the prediction of mechanical properties of nanocomposites

M. Quaresimin, M. Zappalorto, M. Salviato

University of Padova, Dept. of Management and Engineering, Stradella S. Nicola, 3 36100 Vicenza, Italy marino.quaresimin@unipd.it

ABSTRACT. In the recent literature great attention has been paid to the prediction of mechanical properties of polymer nanocomposites, however a comprehensive evaluation of the available mechanical models has not been presented yet.

In this work we propose and discuss a classification of the available modelling strategies into three groups, depending on the scale used to address the problem: micro-mechanical, nano-structural and molecular models.

The inadequacy of micromechanical models on predicting mechanical properties of nanocomposite is quite clear, since they make use of relationships developed for the microscopic scale. On the other hand, nanostructural models, while treating polymer matrix and nanofillers as continuum media, attempt to account for the nanostructure of fillers and its global impact on macroscopic properties.

However, the molecular interactions between nanofillers and the polymer chains of the matrix may also play an important role in the global observed mechanical behaviour. These interactions are accounted for only by the molecular models.

Most of the above mentioned models are mainly focused on the elastic properties of nanocomposites, whilst analytical formulations for toughening mechanisms accounting for the typical features and mechanisms of the nanoscale are still missing.

Some of the existing toughening models will then be modified, according to the experimental evidence, in order to make them size-dependent. Accurate results will be presented and discussed.

KEYWORDS. Nanocomposites; Modelling; Elastic properties; Toughening.