Quantifying Nanoparticle dispersion in polymer nanocomposites using TEM micrographs

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Polymer nanocomposites potentially exhibit superior properties as compared with conventional polymer materials. It is well known that nanoparticle dispersion plays an important role on the material's performance. Transmission Electron Microscope (TEM) is the "golden standard" in nanoparticle dispersion characterization. Quantitative evaluation of nanoparticle dispersion based on TEM micrographs is in high demand for sample comparison and quality control purposes. Existing dispersion quantification methods take a TEM micrograph as a cross section of the specimen, although the micrograph is in fact the projection for a 3-dimensional thin section (~50nm thick) of the specimen onto the imaging plane. This paper intends to investigate the potential impact that the projection view of the TEM micrographs may bring to the quantification of nanoparticle dispersion via existing methods. First, a spatial hardcore model is proposed as the reference model under which nanoparticles disperse ideally and is compared with the previously used homogeneous poisson model. Second, the sensitivity of various dispersion measures to the thickness of the thin section is explored. It is found that the quadrat skewness and the K-function are relatively robust to misspecification of the section thickness and are chosen for further analysis. Third, evaluations are made on the power for detecting clustering and the ability to quantify clustering degrees based on the two chosen measures. Further, the p-values of the test for clustering based on the corresponding dispersion measures is

proposed to quantify the dispersion quality, which can be used across different thickness and particle loadings, and thus can be used for sample comparison or correlation. Finally, an application to real TEM micrographs is used to illustrate the methods.

Key Words: Polymer nanocomposites, TEM, dispersion, spatial hardcore model