STRESS DISTRIBUTIONS AROUND RIGID NANOPARTICLES

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Abstract. A closed form solution for the stress fields around a rigid nanoparticle under uniaxial tensile load is provided. The work explicitly accounts for the presence, around the nanoparticle, of an interphase of thickness comparable to the particle size and different elastic properties from those of the matrix. The solution allows one to determine, in closed form, the stress concentration around nanoparticles relevant for fracture and strength assessments of polymer nanocomposites.

Keywords: nanoparticles, stress concentration, interphase.

1. Introduction

In nanomodified polymers, as the filler size is decreased to the nanoscale, intra- and supra-molecular interactions lead to the emergence of an interphase whose properties differ from those of both constituents and whose thickness may be comparable to the particle size. Sevostianov and Kachanov (2006, 2007) showed that the effect of such interphase on the overall properties may be substantial, the controlling parameters being the ratio of the interphase thickness to the particle size and the variability of the properties across the interface thickness.

The calculation of the stress concentration around a particle embedded within a matrix has been dealt with by many authors, but there are only few works considering interphases. The aim of the present work is to fill this gap and to determine the stress fields around a rigid nanoparticle under uniaxial tensile load. The work explicitly accounts for the presence of an interphase around the nanoparticle, of thickness comparable to the particle size and whose elastic properties differ from those of the matrix. The solution allows one to determine, in closed form, the stress field around the nanoparticle.

2. Analytical framework

2.1 Stress field solution

Let consider a rigid spherical nanoparticle of radius \( r_0 \) embedded by a spherical shell-shaped interphase of radius \( a \), both of them being enveloped into a infinite matrix.
(figure 1a). The matrix and the interphase are elastic, homogeneous and isotropic materials and the interphase has elastic properties different from those of the polymer matrix. This system is loaded by a remotely applied uniaxial tension along direction $X_2$ (figure 1a).

The solution for the displacement field around a particle embedded in an infinite and elastic body loaded by axisymmetrical loads was derived by Goodier (1933) and Oldroyd (1953). Lauke et al. (2000) later analysed the problem of a coated particle embedded within a matrix and noted that, with reference only to the deviatoric part of the elastostatic solution, the displacement fields for each sub-dominion of such a problem can be sought in the following form (Lauke et al., 2000):

\[
\begin{align*}
  u_{r,k} &= \left[ \frac{r^3}{14} a_k + \frac{3\lambda_k + 5G_k}{12\lambda_k r^2} b_k + rc_k - \frac{3d_k}{2r^4} \right] \left( 3\cos^2 \theta_2 - 1 \right) \\
  u_{\theta,k} &= \left[ \frac{5\lambda_k + 7G_k}{14\lambda_k} r^3 a_k + \frac{G_k}{2\lambda_k r^2} b_k + 3rc_k + \frac{3d_k}{r^4} \right] \cos \theta_2 \sin \theta_2
\end{align*}
\]  

(1a) (1b)

where subscript $k=m,a,p$ denotes the sub-domain (matrix, interphase and nanoparticle) and $r$ and $\theta_2$ are coordinates shown in figure 1b; $G_k$ is the shear elastic modulus and $\lambda_k$ is Lame’s constant.

Hence the components of stresses due to the deviatoric part of the remotely applied uniaxial stress can be written as:

![Figure 1. Spherical nanoparticle embedded in a shell-shaped interphase zone under unidirectional load (a). Polar coordinate system used to describe the stress field around the nanoparticle (b).](image)