Predicting Effective Elastic Properties of SU8/ZnO Nano-composite Using COMSOL Multiphysics® Software

K. Das[1], N. Mishra[1]

[1]Indian Institute of Technology Bhubaneswar, Bhubaneswar, Odisha, India

Abstract

SU8 photoresist reinforced with ZnO nanostructures has potential to be widely used as structural component in energy harvesting micro/nano devices. An accurate estimate of the mechanical properties of such a composite is essential for the design of new generation of micro/nano system technologies which can harness the piezoelectric properties of ZnO. Prediction of effective mechanical properties of composite material is a fundamental problem of material science. The first step toward this estimation of mechanical properties is the prediction of the effective elastic properties of the composite. The effective elastic properties of a multi-phase material depends on several factors: (a) elastic properties of the individual phases, (b) geometry and orientation of the reinforcement phases, (c) distribution of the reinforcement phases in the matric phase, and (d) load transfer between the matrix and the reinforcement phases.

Several analytical/semi-analytical solutions exist which predict the properties of unidirectional continuous as well as discontinuous composites, for example Voigt-Reuss, Halpin-Tsai, and Eshelby-Mori-Tanaka micromechanics. However these analytical/semi-analytical methods do not incorporate the spatial distribution of the reinforcement phases in the matrix. Another method/tool to predict the elastic properties is the Finite Element Method (FEM) which allows one to consider a representative volume element (RVE) using which effects of the distribution of the reinforcement phase(s) and effects of matrix/reinforcement inter-phase on the effective material properties of a composite can be studied.

In this work the effective elastic properties of a SU8 photoresist matrix reinforced with ZnO nanomaterial (in the form of cylindrical nanowires, spherical and ellipsoidal particles) have been evaluated employing COMSOL Multiphysics® software. The Solid Mechanics physics of the Structural Mechanics Module is used in this work for the stationary study of a 3 dimensional RVE. The RVE is 1 μm × 1 μm × 1 μm in size which is further reduced to one-eighth due to the presence of reflectional symmetries. A set of homogeneous displacement boundary conditions are applied to the unit cell and meshing done is physics controlled with a minimum element size of 0.269 μm. The post processing of the model is based on the classical homogenization theory in which average stresses and strains are calculated over the entire volume to compute the effective properties. Components of the effective stiffness matrix of the nano-composite along with different elastic properties such as longitudinal elastic modulus (E1), transverse elastic modulus (E2), axial shear modulus (G12) and transverse shear modulus (G23) are obtained for

different volume fractions of reinforcement material ranging from 0.1 to 0.75. This model is validated with certain other composites such as Aluminum/Boron and Epoxy/Graphite for which elastic properties are available from experiment. The effect of various parameters such as volume fraction, continuity, shape, orientation, and distribution of the reinforcement on the effective elastic properties of the nano-composite has been studied and also comparison has been made between the elastic properties obtained by using COMSOL Multiphysics® software with that of existing analytical/semi analytical methods. Figure 1 shows the deformation of the unit cell after applying boundary conditions for calculation of different elastic properties.

Figures used in the abstract

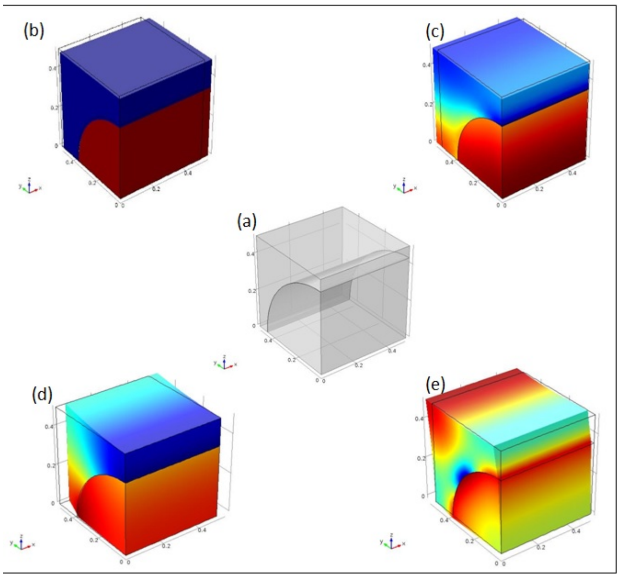

Figure 1: Deformation of the RVE after applying boundary conditions for (a) un-deformed unit cell and deformed unit cell for the calculation of (b) E1, (c) of E2, (d) of G12 ,and of (e) G23. The colour-shades represent the stress distribution.