Molecular Simulations of Epoxy Resins with Water Ingress

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Epoxy resins play a crucial role in today's modern society. Thermosetting epoxy resins are widely used as adhesives, composites and laminates. This is because of their good thermal, chemical, physical, electrical, and mechanical properties, combined with satisfactory processing characteristics. Due to these excellent properties, epoxy materials have found a wide range of applications in various industries such as aerospace, automotive, shipbuilding, building construction, micro-electro-mechanical systems (MEMS), etc. [1] It is well recognized that epoxy resins can suffer substantial losses in their mechanical properties due to the absorption of water. The extensive applications of the epoxy resins make it necessary to establish a sophisticated understanding of the structure and their behavior in diverse situations, such as water ingress.

The present work examines the effect of moisture on an epoxy resin system consisting of 64 EPON-862 monomers (diglycidyl ether of bisphenol F - DGEBF) and 32 DETDA hardener molecules (Diethyltoluenediamine). The examined crosslinking degrees are 71% and 92%. All estimations are carried out by using computational methods and computer simulations. To carry out the calculations, 14 water molecules corresponding to 1% wt of the dry system were added to existing models of epoxy resins, with 3786 atoms and 35.04 Å unit cell length [2]. The water content was chosen on the basis that the usual absorption values range from 1-3% wt for epoxy resins [3][4][5]. Water molecules were added using MAPS (Materials and Process Simulation) designed by Scienomics, while the systems were equilibrated using LAMMPS (Large-scale Atomic / Molecular Massively Parallel Simulator). The Dreiding-X6 force field was used to perform the simulations. For each examined crosslinking degree, three different configurations were made, in which the water molecules were placed at random locations. The bulk modulus B was calculated using the volume fluctuation theory. The glass transition temperature was estimated via a volumetric method, which involves a cooling process in LAMMPS. Based on these simulations, the temperature dependence of the density was plotted and from the break of the slope T_g was estimated. An appropriate algorithm was also developed in MatLab for the above procedure. Finally, for the extraction of Young's modulus and Poisson's ratio, stress-strain experiments were performed using LAMMPS.

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