Finite Element Modeling of Anomalous Moisture Diffusion with Dual Stage Model

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Abstract

In this paper, finite element modeling of anomalous moisture diffusion using commercial finite element code is developed. The modeling method and numerical implementation is based on a dual stage model with both stages described by Fickian terms mathematically. The method is also extended to desorption process at reflow, in which the permanently trapped moisture content is a function of temperature. This paper details the finite element modeling implementation steps for both moisture absorption and desorption. The results are compared to the analytical solutions, and are also compared to the experimental data. A single script using ANSYS APDL is developed for the whole process including absorption and desorption phases.

1. Introduction

The moisture absorbed by a polymer occurs in two states, mobile and bound [1, 2]. In the mobile state, water molecules from the environment migrate to the microscopic pores, free volumes, or voids in the material to achieve concentration equilibrium. The process is similar to a typical mass concentration gradient driven diffusion process, and can be described well by Fick's laws. In the bound state, the water molecules bind with epoxy resins through hydrogen bonding. Two types of bound water are found in epoxy resins [3], as classified as Type I or Type II bonding, depending on the difference in the bond nature and activation energy. Type I bonding corresponds to a water molecule which forms a single hydrogen bond with the epoxy resin network. This water molecule possesses a lower activation energy a.9(o7 se7(l).7(b(v).7(60,(o)-4]TJ TD -.0077 Tc .08re at)3.9(i)3.w8ree f)5.2w8r
mna

% is the total saturated moisture concentration. As long as the parameters of & 5 á æ % 0 ç á 5 and & 6 á æ % 0 ç á 6 are known from experiments, the non-Fickian behavior can be solved by two separate Fickian diffusions using finite element analysis.

For subsequent desorption analysis, if there is a permanent residual moisture in material, it is reasonable to assume that $C_2 = C_r$ (constant) with $D_2 = 0$, indicating the bound water will not be removed from the material. In this case, Equation (2) becomes

% T á; P L 5 %k T á 5 P æ % 0 ç & 5 E å % (4)

It is noted that in Equation (4), if C_r is known, equation (4) becomes a single-stage Fickian type diffusion, so-called modified Fickian diffusion model in [4,11].

Desorption at a higher temperature may remove the bound water completely. In this case, Cr = 0 in Equation (4). A Fickian diffusion process may then be assumed.

3. Diffusion Material Properties

The moisture absorption and desorption behavior of the epoxy molding compound (EMC) samples were studied experimentally [5]. The EMC samples of 1 mm thick with a 50 mm diameter disk were tested at 85°C /85% RH for 10 days, then subjected to 85°C /0% RH desorption for 12 days. The dual stage fit for both absorption and desorption are shown in Figure 1, and Table 1 list the values of diffusivity and moisture concentration for both absorption and desorption. Several important observations are made: 1) non-Fickian diffusion is much slower than Fickian diffusion, which is reflected from the values of D_1 and D_2. 2) The non-Fickian moisture diffusion contributtfusio7.09 Tc .395 Tw rcon3x,1.9(r)4.5( )]TJ 0 -1.1437 TD -.09q75.68D -.09fTJ 1.35f .395 3(e fi)0 software for transient heat analysis can be effectively used for transient moisture diffusion modeling. For a non-Fickian moisture diffusion process, two separate Fickian diffusion analyses are performed first using the dual-stage model parameters. A single script with ANSYS APDL is developed to perform the anomalous moisture diffusion automatically. If a desorption process is followed, and the residual moisture content is considered, the script can continuously perform the diffusion modeling correctly. As an example, a two dimensional finite element simulation to characterize the dual stage moisture absorption and desorption of a thin plate sheet of dimension 50mm x 1mm is conducted. Figure 3 shows the comparison between finite element results and analytical model results in terms of the total mass of moisture content as

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