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Experimental validation of molecular modeling of crosslinked polymers applied in electronic packaging

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ABSTRACT

Moore Law (double number of transistors in a chip in every 18-24 months) has a big influence on microelectronics. It apply well for memories and microprocessors, but there are other application like radio frequency devices (RF), power management subsystems, passive components, biochips, sensors, actuators and MEMS, which have big impact on semiconductor industry. Those diversified technologies are known as “More than Moore”. New materials are introduced all the time and assessment of their properties is essential from technical point of view. In electronic packaging epoxy resins gain field and became more and more popular in usage. Fast and cheap way of assessing thermo mechanical properties of epoxy resins are advanced computing methods like molecular modelling. Despite all the advantages of modelling its gives only approximated result. It is not a precise value rather a trend, so experimental validation of results is mandatory. The authors created a molecular model of a cross-linked network of a EPON 862 resin and a TETA hardner. The change of density in function of temperature were assessed. The glass transition and coefficient of thermal expansion was calculated. The authors built measuring setup which allow them to validate the molecular simulations. The Set Up is based on Archimedes principle. The sample is placed in a jar with oil and is heated to certain temperature. During heating the weight is changing. For preliminary test SIQ resin was used, the glass transition and coefficient of thermal expansion was assessed. Experimental and literature results are convergent. The set up is credible so the results of molecular simulation can be validated by it.

Key words: molecular modelling, cross-linked polymers, epoxy resin

1. INTRODUCTION

“Moore Than Moore” is a extension of Moore Law but it describes other technologies then memories and microprocessor. Other like radio frequency devices (RF), power management subsystems, passive components, biochips, sensors, actuators and MEMS. New materials are introduced all the time, so assessment of their properties is essential. In electronic packaging the usage of epoxy resins is growing. One of the approach of assessing thermo-mechanical properties of resins is advanced computing methods like molecular modelling.

2. MOLECULAR MODELING

The authors created a molecular model of a cross-linked network of a EPON 862 resin and a TETA hardner. In the figure 1 cross-linked system is presented and on figure 2 resin and hardner. The change of density in function of temperature were assessed (Fig. 3). The glass transition and was calculated, it was close to the literature data. We cannot forget that advanced computing methods gives only approximated results so experimental validation is mandatory [1, 2, 3]. For this purpose the authors built measuring set up.

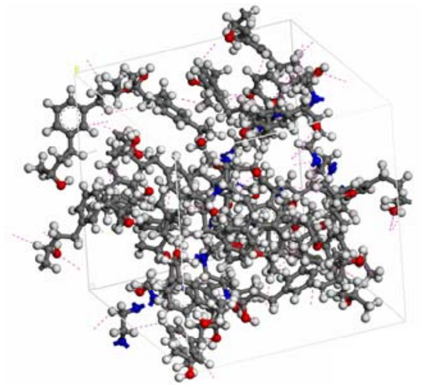

Fig. 1. Cross-linked network of resin and hardner

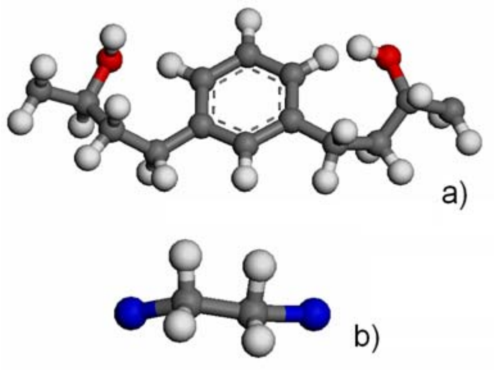

Fig. 2. Resin (a), Hardner (b)

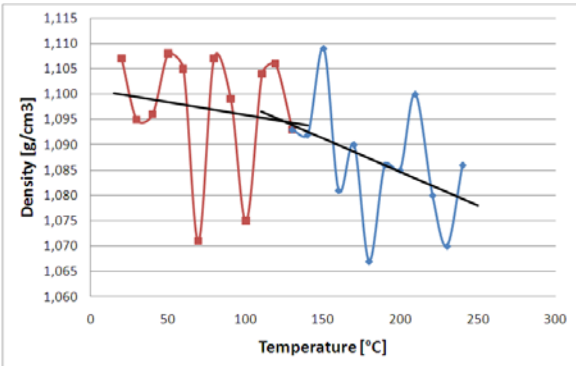

Fig. 3. Density in the function of Temperature – molecular simulation

3. THE IDEA OF MEASURING SET UP

The Set Up is based on Archimedes principle [4], which says the buoyant force on a submerged object is equal to the weight of the fluid displaced or as in equation (1).

$$F_B = \rho_f V g \tag{1}$$

Where F_B is the buoyant force, ρ_l the density of a fluid, V volume of the object, and g acceleration of gravity.

To obtain sample density it is needed to measure sample in the air and in the fluid of known density. When sample is measured in the fluid its weight is partly equilibrate by buoyant force so the balance shows ostensible weight. The density of a sample is given in equation (2).

$$\rho = m / V \tag{2}$$

Where ρ is the density of a sample, m the weight of the sample, V volume of the sample. According to Archimedes principle the volume of the sample is given with equation (3).

$$V = (m - m_o) / \rho_f \tag{3}$$

Where V is a volume of the sample, m the weight of the sample, m_o ostensible weight, ρ_f the density of a fluid. Using equation (2) and (3) we have equation for density of a sample (4).

$$\rho = (\rho_f * m) / (m - m_o) \tag{4}$$

Where ρ is a density of a sample, ρ_f the density of a fluid, m the weight of the sample, m_o ostensible weight. Knowing the density of a fluid and ostensible weight of the sample we can calculate the density of the sample.

4. MEASURMENT

The Set Up (Fig. 1) is used for monitoring the change of density of epoxy resin in the function of temperature. The small amount of epoxy resin is placed on a very thin TEFLON film, and the epoxy together with the film is immersed in a reservoir filled with mineral oil. The mineral oil is heated by coil-shaped resistance heater. A resistance Pt100 type temperature sensor, together with a PID temperature controller, is used to monitor and control the temperature of the mineral oil. The epoxy resin and TEFLON film are attached to a digital balance by a thin string, so the weight of the epoxy resin can be measured.

Fig. 1. The measuring set up

For the preliminary test SIQ resin was used. A small sample of 4 mm diameter was weighted in the air. Next as mentioned before the sample was placed on boat-shape TEFLON film and submerged into mineral oil. The measurment started from 80ºC with step of 10ºC. At every step there were few minutes for stabilizing the indictation of the balance. The ostensible weight from every step was collected. Using equation (4) the density in every step was calculated. Figure 2 presents density in the function of temperature for measured resin. The measured value of Tg is converged with literature data.

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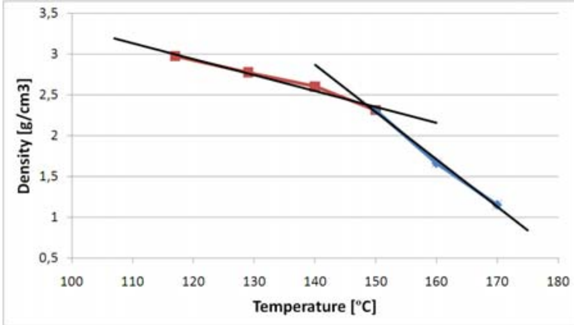

Fig. 2. Change of density in the function of temperature for SIQ resin

5. SUMMARY

The Set Up based on Archimedes Principle for assessment of change of density in the function of temperature was designed and built. Preliminary measurements of known resin were preformed. The results are converged with the literature study. The Set Up is credible for validation of molecular modelling.

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