Numerical and experimental assessment of moulding compounds thermo mechanical properties

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Usage of polymers material in microelectronic is common. Assessment of their properties is essential. Advanced computing methods gives cheap way of achieve it. Experimental approach complement it.

Key words: molecular modeling, mesoscale, moulding,

1. Introduction

Usage of polymers material in microelectronic is common. For electronic packaging polymers are used as: encapsulants, underfilers, moulding, material for Printed Circuits Borads (PCB), adhesives and many more /1/. Properties assessment of those polymer materials is vital /2/. One of the cheapest way is to use advanced computing methods. Molecular and Mesoscale simulations give such possibility. The Authors create a model of EPON 862 (resin) and TETA (hardner) in Materials Studio (MS) software of Accelrys.

2. The Model

The methodology of creating a model is based on /3, 4/. Resins and hardners are connected using self written Perl language script. Hardner and resins are put together in random position in 3D Periodic Cell. If the head and tail atom are in close contact they are connected. This step take so long as there are no more free resin and hardner. Next step is to change back the charge of the atoms, and check for artefacts (connection that cannot occurred in nature). The figure 1 presents algorithm of the connection.

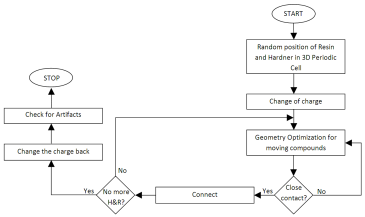

Figure 1: Algorithm of connecting resin and hardner

Figure 2 presents ready model and idea of the 3D Periodic Cell. When the end of compound leaves for example left wall, it will appear going into the cell from right wall. So the cell is surrounded with it virtual copies.

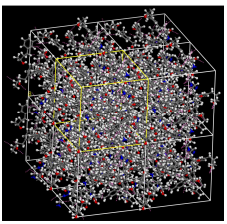

Figure 2: Ready model and idea of 3D Periodic Cell

The structure is artificial, so the length, the angles between the atoms are not like in reality. So it has to forget it history in order to be less artificial. One of the way

is to supply energy into the system (anneal). The procedure uses one of MS module – Forcite. The annealing is done in 600K for 1 ns. Next the temperature is decreasing to 300K. The structure is ready for calculation.

3. Molecular & Mesoscale modeling

The change of density in the function of temperature where calculated using algorithm presented in figure 3.

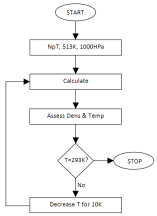

Figure 3: Algorithm of density assessment

The Forcite module is used again, Molecular Dynamics NVT (constant: Number of atoms, Volume, Temperature) is used. The starting temperature is 513K, every step is 200 ps long. The temperature changes in the rate of 10K till 293K. From the graph (figure 4) the glass transition (Tg) could be assess.

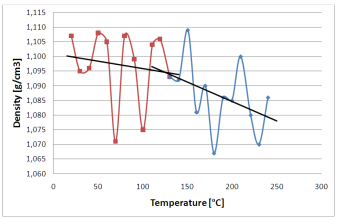

Figure 4: Change of density in the function of temperature

As it can be seen from the graph the Tg could be somewhere near 120°C, but the fluctuation of density are rather big.
To make mesoscale simulation, one additional step is necessary. The molecular model must be converted into mesoscale. The idea of changing is based on converting a group of atoms into one bead. The size of bead should be appropriative, if the bead is too big the results are less accurate, if the bead is too small the simulation last longer and the whole idea of converting do not have sense. It is important not to split functional group. The authors made an experiment how bead size influence the results of simulation. And for EPON862 and TETA, the best bead size is presented in figure 5.

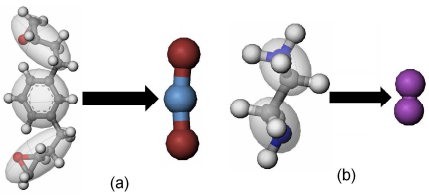

Figure 5: Changing into beads: (a) resin, (b) hardner

For mesoscale the Mesocite module form MS is used for simulation. The algorithm of density assessment is very similar to algorithm presented in figure 3. Figure 6 presents change of density in the function of temperature.

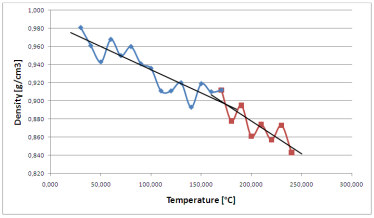

Figure 6: Change of density in the function of temperature for mesoscale

The fluctuation of the density are much smaller in mesoscale than in molecular approach, but as it can be seen from the figure 6 there cannot be observed inflec-

tion point. Mesoscale simulation need to be adjusted.

4. Experimental approach

For evaluation of the results the authors built a measuring Set Up based on Archimedes Principle. It says that any object, wholly or partially immersed in a fluid, is buoyed up by a force equal to the weight of the fluid displaced by the object (equation 1) /5/.

$$F_B = \rho_f \cdot V \cdot g \qquad (1)$$

Where F_B is the buoyant force, ρ_f the density of a fluid, V volume of the object, and g acceleration of gravity. Knowing the density of a fluid and ostensible weight of the sample we can calculate the density of the sample (equation 2).

$$\rho = (\rho_f \cdot m)/(m - m_o) \qquad (2)$$

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. Figure 7 presents measuring set up.

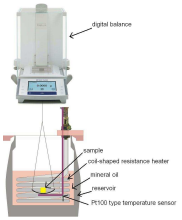

Figure 7: The measuring set up

The algorithm of measurement is presented in figure 8. The measurement starts from 80ºC, the temperature of mineral oil must be stable, then the ostensible weight is assess, the temperature is increased for 10ºC and it must be stable, and next ostensible weight is assess. The measurement ends at 170ºC.

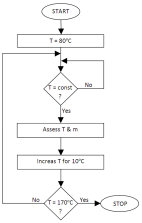

Figure 8: The measuring set up

The figure 9 presents change of density in the function of temperature for SIQ resin. The inflection point (Tg) is near 147ºC and it is converge with the literature data. The measuring set up is credible so it can be used for validation of molecular and meso simulations of polymers materials.

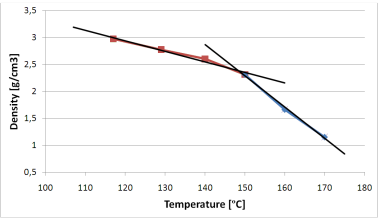

Figure 9: The change of the density in the function of temperature for SIQ resin

4. Summary

The authors present in this paper numerical and experimental approach for assessment of thermo mechanical properties of moulding compounds on example of EPON862 and TETA. Molecular modeling allow to assess other properties of examined materials such as i.e. Young modulus. Results of molecular simulation are converted with literature data but the fluctuation of the density is quite big, so more effort must be made for improving the results of simulation. Results of mesoscale simulation have less fluctuation but no inflection point could be ob-

served. More work is still needed for adjusting the simulation parameters. It is important to remember that advanced computing methods do not give precise value, rather a trend of the examined property. For this reason experimental validation of simulation is mandatory.

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