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<tr>
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Abstract:
In this work, the possibility of laser aided curing of GnP/epoxy nanocomposites is explored by means of finite element analysis. A multi-scale and multi-physics analysis is performed to identify and optimise critical manufacturing parameters –laser speed and power. The proposed model is parametrically studied and its results are thoroughly discussed in terms of polymerisation degree and temperature field depth. Finally, the laser scanning of a specimen was conducted and the polymerisation performance was recorded.
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Keywords: graphene nanoparticles, polymer, nanocomposite, laser, polymerisation, multi-scale, finite element analysis

1 Background

The manufacturing process of any composite material structure exhibits important challenges, including the development of time and cost effective methods, enabling mass production with high repeatability in the products’ specification. The ability of the carbon-based nanofillers to absorb light wavelengths could be exploited in eco-friendly manufacturing processes based on radiation and laser curing techniques. Especially, graphene is a two-dimensional material with carbon atoms in a honeycomb lattice. It has many potential applications thanks to its unique electrical, mechanical, chemical and optical properties [1–3]. The optical transmittance of multilayer graphene films up to 65 layers thick was studied in the work of Zhu S. E. et al. [4], finding the optical transmission through graphene films in the visible region be solely determined by the number of graphene layers. The incorporation of periodic gold nanoparticles arrays into graphene-based photodetectors to enhance and tune light absorption of graphene was found in the work of Zhu J et al. [5]. The significance of the ability of graphene to absorb the light was highly utilised by direct absorption solar collectors (DASCs) used in solar energy conversion applications [6–8].

Furthermore, laser applications have received an increasing attention for a wide variety of applications such as scientific, military, medicine, industries and other fields due to its excellent quality with high productivity and flexibility [9]. Main variable parameters in this process are the power and diameter of the laser beam as it moves across the surface of a workpiece. A number of models have been developed to simulate the laser treatment of a surface and study the effect of the process variables and the quality of the product. A three-dimensional finite element modelling of laser surface modification is presented in the work...
[10], while in project [11] a three-dimensional numerical heat transfer model was employed to simulate the laser structuring of polymer substrate material in the Three-Dimensional Molded Interconnect Device (3D MID) which is used in the advanced multi-functional applications. In terms of graphene ability to absorb light, it is combined with laser heating in the simulation of the next study [12]. In specific, it investigates heat transfer on the multi-layered structure with graphene overcoat induced by laser heating.

Knowledge from all these seemingly irrelevant works has been combined to form a multi-scale finite element model to simulate the curing of graphene/polymer nanocomposite. At first, a unit cell consisting of the GnP particle and the liquid epoxy is considered to determine the temperature dependent thermal conductivity and specific enthalpy. Afterwards, a macroscopic specimen, on which the unit cell obtained properties are distributed, is subjected to laser loading conditions and the effect of the laser speed and power on the polymerisation degree and temperature field depth are found. Considering all the selected data, it will be shown that the polymerisation degree and the penetration of the temperature field increases with decreasing laser speed and increasing laser power, forming a scheme of highly customised manufacturing process in accordance to the specimen thickness and production line rate.

2 Multi-scale finite element model

The unit cell is a square plate consisting of the GnP particle and its surrounding liquid polymer. Between the GnP and the polymer, thermal contact elements were applied, simulating the interfacial thermal resistance (Figure 1(a)). The geometry was built with SOLID70 3D 8-node thermal solid elements. The interfacial resistance was modelled through CONT174 – 3D 8-node surface to surface contact element- and TARGE170 – 3D target segment - and it was approached by a temperature dependent Kapitza resistance. For both phases, temperature-dependent properties were assumed. For the case of epoxy, the specific reaction enthalpy of a two-component resin (Biresin CR170/CH150-3) was modelled for temperature rate of 1K/min as recorded [13]. The thermal conductivity exhibited the same trend as the specific reaction enthalpy with K=0.06W/mK when the polymerisation degree is 0 (liquid) and K=0.19W/mK when the polymer is fully polymerised (solid). Accordingly, the applied response for GnP was retrieved by the work [14]. The temperature-dependent thermal properties were obtained at this level, to be afterwards distributed in the specimen model.

The specimen is a rectangular cuboid with length of 10mm, width of 5mm and thickness of 1mm (Figure 1(b)). It was built with SOLID70 3D 8-node thermal solid
elements. Temperature-dependent material properties, previously obtained in the unit cell, were distributed randomly in the specimen volume, to approach the nanocomposite architecture. The initial temperature was set to the room temperature (20°C). To simulate the heat offered by the laser, the laser beam was modelled as a heat flux (heat rate per area) applied on a circular area with radius $r_{\text{laser}}=200\mu m$. The maximum laser power was 1.25W and the laser speed ranged between 5mm/s and 300mm/s. On the rest area – which is the area not being loaded with the laser heat flux- convection was applied to simulate the cooling of the surface of the rest material. The convection coefficient was set to 10W/m²K (-air of with zero flow velocity) while the room temperature was set to 20°C.

3 Results

A parametrical study was conducted on the effect of laser parameters (speed and power) on the polymerisation degree obtained and the depth of the temperature field. In each case, a single scan on the length of the specimen was applied. The polymerisation degree is presented in function of the position of the laser $x$. The coordinate system is set to the middle of the specimen.

In Figure 2, the effect of laser parameters (speed and power) on the polymerisation degree of nanocomposites with weight fractions of 5% is presented. In every case, the polymerisation degree is increased with laser power as a result of increased offered heat. On the other hand, the polymerisation decreases with laser speed. When the laser beam scans quickly the specimen, smaller amount of heat per area is offered compared to slower scans, therefore leading to lower polymerisation degree.

One of the most crucial manufacturing parameters is the temperature field depth achieved, deciding the thickness of the final product. The effect of the laser power and speed on the temperature field depth was studied for 1.0-12.5wt% nanocomposites. The depth was decided as the distance from the top/heated surface to the point where the temperature was raised to 5% from the initial one ($\approx 308K$). The through-the-thickness temperature field was measured at the centre of the specimen at the middle of the process. In Figure 3, the obtained results are presented. In Figure 3(a), the depth was recorded for 1.5-50% laser power and laser speed of 5mm/s, while in Figure 3(b) the laser power was kept constant to 1.5%. As expected, the temperature field depth increases with increasing laser power and decreasing laser speed. The maximum sample thickness could be 0.20mm (200μm) when the laser power is 10% and the laser speed is 5mm/s. Considering the above findings, this laser curing process could be efficient for the manufacturing of nanocomposite films and coatings.
Finally, the laser scanning of an area of 1mm x 1mm in the centre of a specimen 2mm x 2mm was conducted. A central area was chosen on the material to avoid any edge effects. The scanning was applied to specimens with different thicknesses – 1mm, 0.5mm and 0.2mm - and the laser had a speed of 5mm/s and power set at 5%, while the nanofluid was loaded with 5wt% GnP. The design of the laser curing would be successful, if by the end of the process the polymerisation degree of the volume/mass would be at 25%.

The polymerisation degree achieved for each case is presented in Figure 4. As it would be expected, the polymerisation degree is increasing with decreasing thickness, while for t=0.5mm the 25% of the specimen was already polymerised. This observation does not necessarily indicate that the scanned area was cured through its thickness, but also the nearby volumes might have been polymerised as a result of the heat transfer. For specimen thickness t=0.2mm, the polymerisation degree reaches 60% indicating clearly the polymerisation of volumes which were not scanned by the laser. For comparison reasons, the specimen with thickness of 1mm was laser cured with pre-heating the material at 40°C. It could be seen that material pre-heating has a minor effect on the polymerisation degree.

4 Conclusions

The laser-aided curing of graphene/epoxy nanocomposites was simulated by a multi-scale finite element model. The temperature-dependent thermal properties were obtained at unit cell and then the polymerisation performance of the material was calculated for different filler loading and manufacturing parameters (laser speed and power). A scheme was created on the customisation of the manufacturing process, accounting for the laser speed and power, and the material thickness. By decreasing the laser speed, the thickness of the polymerised material was increased, while the increase of laser power gave rise to the maximum developed temperature. Finally, it was found that this manufacturing method is suitable for the polymerisation of thin films and sensors.

5 Conflict of Interest

There is no conflict of interest to be declared.

6 References


Figure 1: (a) Unit cell top view with unit cell width $w$ and GnP particle diameter $d_{GnP}=25\mu$m. (b) Cuboid specimen model of nanocomposite with surface of 10mm x 5mm and thickness of 1mm.

Figure 2: Effect of (a) laser speed (b) laser power on polymerisation degree of 5.0wt% GnP/epoxy nanocomposite. The laser power was set to 1.5% for results in (a) and the laser speed was 5mm/s for (b).

Figure 3: Temperature field depth as a function of (a) laser power and (b) speed for 1.0-12.5wt% GnP/epoxy.

Figure 4: Polymerisation degree on scanning area of 1mm x 1mm with different thicknesses and including material pre-heating effect in function of time.
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