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Liquid Crystal Polymer for QFN packaging: Predicted thermo-mechanical fatigue and Design for Reliability

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ABSTRACT

Thermoplastic resins, such as Liquid Crystal Polymers (LCPs), have many attractive properties for microelectronic cavity package manufacturing (in particular low gas permeation and low dielectric constant). In order to reduce anisotropic mechanical properties inducing a potential fragility of the material and then a lack of reliability of the package, various approaches are currently studied in particular the addition of mineral fillers. A dedicated Design of Experiments (DoE) is performed to assess the optimal thermo-mechanical properties of the LCP compound and then the optimal composition of the package leading to the maximum operating lifetime. In this way the long-term reliability of an electronic package (Quad Flat No-lead – QFN – package) based on various formulations of the LCP composite is assessed by thermo-mechanical simulation using Finite Element Method (FEM). A Design for Reliability (DfR) methodology is proposed according to the simulation results based on Taguchi methodology. This methodology allows the determination of the optimal composition (nature/proportion/size/chemical functionalization of fillers) of the LCP package by reducing the number of experimental studies that are very time consuming.

1. Introduction

The development of a new generation of innovative thermoplastics for microelectronics and photonics is essential to make cavity packages able to compete with ceramic packages in terms of weight, cost and design flexibility. Among thermoplastic resins, Liquid Crystal Polymer (LCP) offers attractive properties including low gas permeation, high temperature resistance [1], thermal stability and low dielectric constant (3.1 at 1 MHz and 2.8 at 10 GHz [2]). However LCP presents anisotropic mechanical properties [3] inducing a discrepancy in Coefficient of Thermal Expansion (CTE) and Young's modulus values and then a potential fragility of the material that can lead to problems of sustainability and therefore reliability of the package.

Various approaches are currently studied to reduce LCP anisotropy in particular the addition of mineral fillers. Silicon dioxide (SiO_2) is commonly used as additive compound because it improves mechanical properties of polymers and has a low dielectric constant [4]. However agglomeration of fillers affects the dispersion into LCP. An original approach consists in a chemical functionalization of SiO_2 particles to enhance the dispersion and the stabilization of the SiO_2 particles in the LCP matrix. In a previous study [3], we have demonstrated that the addition of functionalized SiO_2 particles seems to reduce the formation of clusters into precipitated LCP whatever the particle size, leading to a better distribution and then a less anisotropic material. The choice of the size of SiO_2 particles, the nature of the chemical function or also the filler content will determine the CTE and Young's modulus of the LCP composite and then the reliability of the package. Therefore, to assess the optimal composition of the LCP composite for a reliable package is problematic.

Reliability assessment is essential to validate the performances of electronic components and enlarge their dissemination. In this context, Design for Reliability (DfR) concept is an effective way to improve the design and manufacturing stages allowing predictive modeling to better understand the physics of failure and to predict the probability of field failures [5,6,8].

In the literature few results are reported on LCP package reliability. Previous studies showed a higher reliability of such QFN package compared to QFN based on overmolding compounds [8,9]. In this paper, a dedicated Design of Experiments (DoE) is performed to assess the optimal thermo-mechanical properties of an LCP package leading to the

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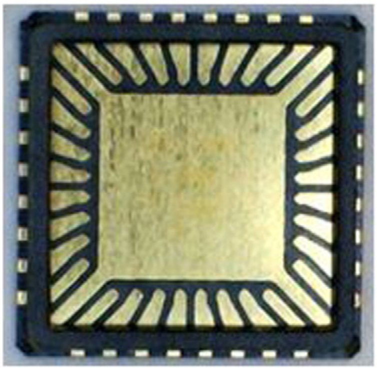

Fig. 1. Picture of a QFN 7 × 7 cavity package (7 × 7 mm^2).

maximum operating lifetime. In this way 3D thermo-mechanical simulations based on the Finite Element Method (FEM) using ANSYS software are performed to predict lifetime of the solder joints that are the critical areas in terms of package reliability. Simulation results are then processed according to the Taguchi methodology to determine optimal thermo-mechanical properties of the LCP composite and then the optimal composition for LCP electronic packages.

The purpose of the present study is then twofold:

- reduce the LCP anisotropy by adding functionalized SiO_2 particles,
- determine the ideal composition of the LCP compound for electronic packaging applications using a methodology based on thermo-mechanical simulation leading to the maximal lifetime of the LCP package. This methodology allows to considerably reduce the number of experimental studies that are costly and time consuming.

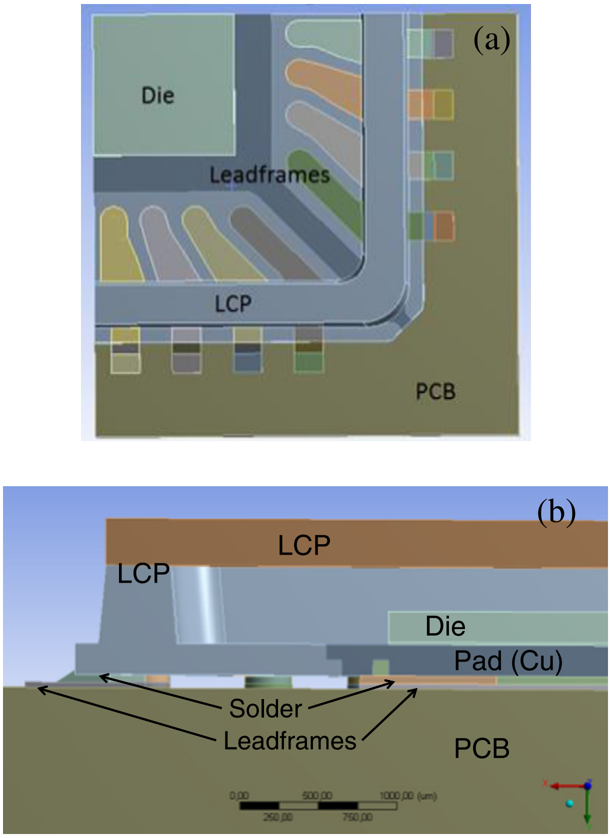

Fig. 2. (a) View of the model type “quadrant” applied to the QFN package and (b) view of the cross-section of the package.

Table 1
QFN package dimensional characteristics.

Parameters	Dimensions
Die size	3 × 3 mm^2
Die thickness	0.2 mm
Package size	7 × 7 mm^2
Leads width	0.3 mm
Leads number	32
Pitch leads	0.65 mm
Solder joint thickness	5 μm

2. Finite Element Analysis fatigue model

In this study a Quad Flat No-lead (QFN) cavity package based on LCP composites is addressed (see Fig. 1). The attractiveness of this package type is due to both its compactness and good power dissipation.

A QFN 7 × 7 cavity package mounted on a circuit board is considered.

Several solder joint fatigue lifetime models are described in the literature [10]. The well-established model of Sn96.5Ag3Cu0.5 solder joint fatigue based on Darveaux's methodology leading to strain energy density estimation is used [11,12]. This model allows to describe the creep behavior and the viscoplasticity of the solder alloy subjected to strain during temperature cycling when the package is mounted on board. According to this methodology and Finite Element Method (FEM), 3D thermo-mechanical simulations are performed using ANSYS software (Ansys Workbench version 14.0 [10]) to predict the lifetime of the solder joints of different composition of LCP packages.

2.1. Package geometry

Due to QFN package symmetry, only ¼ of the assembly is modeled (see Fig. 2). Simulations are then performed on a “quadrant” section of the QFN to reduce the calculation time. The fixed node is located on the vertex below the “quadrant” section of the QFN (PCB side) (Table 1).

A refined hexahedral meshing is performed in the solder joints as shown in Fig. 3. A thinner meshing is carried out on the solder joints that are the critical areas in terms of reliability. The model has 1,540,441 nodes and 763,903 elements. Elements are mainly hexahedral and tetrahedral.

2.2. Package material properties

The eutectic solder SAC 305 (Sn96.5Ag3Cu0.5) is a lead-free alloy. Anand's constitutive model takes into account the visco-plasticity behavior of the solder material and its creep. The properties of the solder

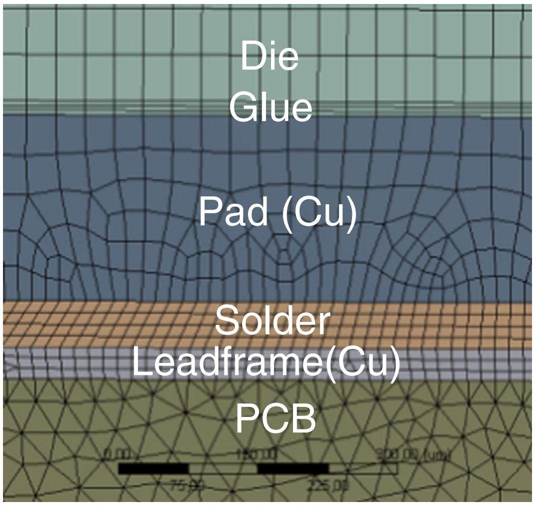

Fig. 3. Cross-section of solder joint with hexahedral fine mesh.

Table 2
SAC 305 parameters in Anand's viscoplastic model.

Parameters	Values
S_0 [MPa]	45.9
Q/R [K]	7460
A [1/s]	$5.87 \cdot 10^6$
ξ	2.0
m	0.0942
h_0 [MPa]	1375.98
s [MPa]	58.3
n	0.015
a	1.5

joints required for simulation are extracted from the literature (see Table 2) [12]. Thus the solder joint fatigue is calculated during the thermal cycles.

CTE and Young's modulus of SAC 305 are given in Table 3. Silicon and copper are assumed to be linear elastic and their properties (CTE and Young's modulus) to be temperature independent (Table 3) contrary to glue that is considered as temperature dependent (Tables 4 and 5).

The properties of the thermal glue (epoxy-type) are given in Table 4.

The FR4 PCB properties take into account anisotropy (see Table 5). The properties before glass transition temperature are considered.

2.3. Thermal cycling

Thermal cycling consists in a sequence of high and low temperature portions to trigger the initiation and propagation of thermo-mechanical fatigue cracks in solder joints. Fig. 4 plots the experimental thermal cycling profile implemented in FEM simulations: [−65 °C, 145 °C]. Temperature is applied on each node of the model.

3. Solder joint fatigue model

Darveaux's model is the most used energy-based model for solder joint fatigue lifetime. The methodology is based on Anand's parameters to carry out the FEM calculation of the volume-averaged accumulated strain energy density (SED) per cycle. With the Darveaux's parameters, solder joint lifetime can be calculated using the following equations [16]:

$$N_0 = K_1 \Delta W_{ave}{}^{K_2} \tag{1}$$

$$\frac{da}{dN} = K_3 W_{ave}{}^{K_4} \tag{2}$$

$$\alpha = N_0 + \frac{a}{da/dN} \tag{3}$$

K_1, K_2, K_3 and K_4 are Darveaux's constants related to lead-free alloy material and geometry type [17]. N_0 is the number of cycles before crack initiation. da/dN is the crack growth rate per cycle. ΔW_{ave} is the incremental inelastic energy per cycle in the solder joint volume. N is the total number of cycles before failure. a is the feature crack length, usually equals to pad diameter for BGA or pad length for plane solder joint. α is the characteristic lifetime when 63.2% of the population has failed.

Table 3
Thermo-mechanical properties of silicon, copper and SAC 305 [13].

Materials	Young modulus (Pa)	CTE (ppm/K)
Silicon (die)	$1.31.10^{11}$	1,65
Copper (pad)	$1.24.10^{11}$	1,70
SAC 305 (solder)	$3.77.10^{10}$	25

Table 4
Thermo-mechanical properties of the thermal glue [14].

Glue		
	Temperature (°C)	Values
Young modulus (Pa)	−65	2,833,745
	25	1,399,635
	100	579,159
	150	75,842
	200	58,605
	250	53,089
CTE (ppm/K)	<96 °C	94
	>96 °C	165
Poisson ratio	0.3	

4. Design of Experiments (DoE)

The Design of Experiments (DoE) consists of several combinations of thermo-mechanical properties of the LCP (CTE and Young's modulus). Each combination of parameters is simulated by FEM to obtain strain energy density per cycle of the solder joint for a thermal cycling profile (see Fig. 4). The impact of each parameter on the fatigue lifetime is analyzed. Finally, Taguchi methodology is used to post-process simulation results [18].

4.1. DoE methodology

The main LCP mechanical properties are considered: Young's modulus and CTE. Three different values of Young's modulus (A = 5.7 GPa, B = 12.3 GPa and C = 20 GPa) and CTE (a = 7.1 ppm/K, b = 10 ppm/K and c = 14 ppm/K) are considered. The first set of values (A = 5.7 GPa and a = 7.1 ppm/K) corresponds to the experimental values obtained for a commercial LCP while the second set (B = 12.3 GPa and b = 10 ppm/K) represents the LCP datasheet values. The latest set of values (C = 20 GPa and c = 14 ppm/K) corresponds to the acceptable boundary values for LCP. Young's modulus values are experimentally determined by tensile testing and CTE values by dilatometry. In a previous study, we have demonstrated that the addition of SiO_2 particles (functionalized or not) significantly reduces the anisotropic behavior of the LCP [3]. Isotropic properties for LCP are then considered in the simulations.

4.2. Simulation results

The different combinations of parameters are simulated as shown in Fig. 3. The main result of simulations is the strain energy density (SED) per cycle in the solder joint. The lifetime is then calculated using Darveaux's methodology [16].

First a Taguchi table called “L9” is proposed considering all the parameter combinations and the simulation results (Table 6). Several “L4” tables are then selected for the post-processing to highlight the interaction between two parameters [19]. The aim is to determine the interaction between each pair of parameters and to extract the optimal value for CTE and Young's modulus. Fig. 5 presents (a) the thermal

Table 5
Thermo-mechanical properties of PCB [15].

PCB	Direction		
CTE (ppm/K)	x	y	z
	15.9	19.1	80.5
Young modulus (Pa)	x	y	z
	$2.24.10^{10}$	$2.24.10^{10}$	$1.6.10^9$
Poisson ratio	xy	yz	xz
	0.02	0.143	0.143
Shear modulus (Pa)	xy	yz	xz
	6.10^8	$1.99.10^8$	$1.99.10^8$

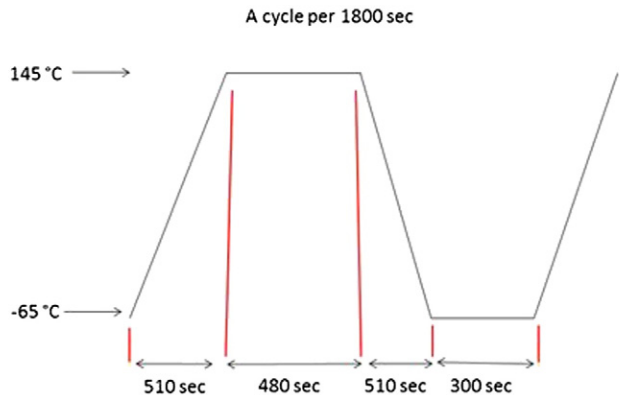

Fig. 4. Thermal cycling profile used for FEM simulations.

cycling/Young's modulus interaction and (b) thermal cycling/CTE interaction.

According to the results, the lifetime decreases with LCP Young's modulus while it increases as CTE is increasing. These observations are in agreement with the literature [20]. When the Young's modulus increases, the LCP becomes more rigid and the solder probably more breakable. When the CTE increases, it tends towards the CTE of the other materials constituting the package. It is well known that a decrease in the difference of CTE between two materials decreases the risk of crack.

4.3. Determination of the optimum LCP composite mechanical properties

Considering these interactions, optimum values for CTE and Young's modulus of the LCP are graphically identified using Taguchi methodology [21,22]. Fig. 6 shows these interactions. Using a dedicated data processing each "L4" Taguchi table allows drawing two straight lines that present the interaction between two parameters. For example in graph (a) the full line presents the variation of the package lifetime in the Young's modulus range [5.7, 12.3 GPa] between two values of CTE, 10 ppm/K and 7 ppm/K, and the dotted line the variation of the package lifetime in the same Young's modulus range but between 7 ppm/K and 10 ppm/K. The intersection of the two straight lines gives the optimal value of the considered parameter (Young's modulus for graph (a)) in the studied range. Graph (b) is similar (i.e. variation of the package lifetime for a given value of Young's modulus in the CTE range of [7.1, 10 ppm/K]). The complete methodology is given in reference [23].

The optimum values are summarized in Table 7.

According to the simulations and the DoE, a maximal lifetime of the QFN package based on LCP seems to be obtained with two sets of values: (8.3 GPa; 8.8 ppm/K). Then, the ideal composition of the LCP compound for electronic package applications must present these mechanical properties.

Table 6
Simulation results.

Parameters		Results
Young's modulus (GPa)	CTE (ppm/K)	α: Characteristic lifetime (cycles)
		QFN 7 × 7 − 32 leads
A = 5.7	a = 7.1	8229
A	b = 10	8699
A	c = 14	9113
B = 12.3	a	7523
B	b	8218
B	c	8943
C = 20	a	6586
C	b	7558
C	c	8628

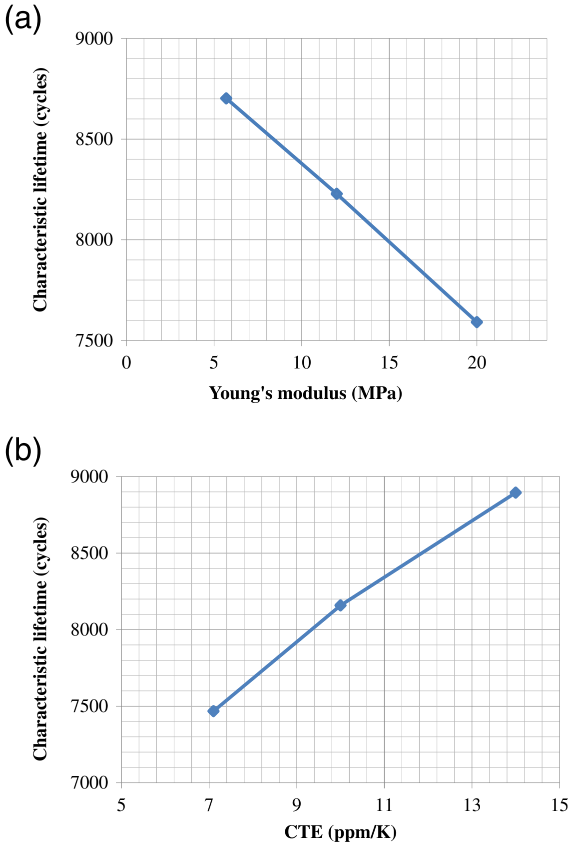

Fig. 5. Taguchi results: (a) Thermal cycling/Young's modulus interaction and (b) thermal cycling/CTE interaction.

5. Mechanical characterization of the LCP composites

Many studies are carried out on the addition of polymers or inorganic fillers to LCP [24] for reducing anisotropy but none on functionalized inorganic particles. A phenyl functionalization is considered in this study because this group is able to create interactions with LCP chains improving the filler dispersion [24,25]. The aromatic groups form π–π interactions that could lead to a better dispersion and compatibility with the LCP matrix.

A Vectra® LCP is provided from Ticona [26]. The fillers are commercial precipitated silicas from Eka Industries: Bindzil 40/170 (20 nm average diameter and 170 m^2/g of specific surface) and Bindzil 30/360 (7 nm average diameter and 360 m^2/g of specific surface). The silica surface is functionalized or not with phenyl groups via a sol–gel process. The fillers are then added to the melted LCP and extruded using a twin screw extruder. A homogeneous mixture is obtained.

Manufactured samples are summarized in Table 8.

The purpose is to determine which LCP composite leads to the expected CTE and Young's modulus values deduced from simulation (Table 4). The influence of the silica particle size and the chemical functionalization on composite Young's modulus and CTE is experimentally studied.

5.1. Young's modulus measurement

Young's modulus measurement is performed using a tensile test tool (Instron 5565). Four tensile test samples based on the samples A, B, C and D have been manufactured according to ISO 527-2 5A standard. Young's modulus is experimentally determined for each sample in the flow direction.

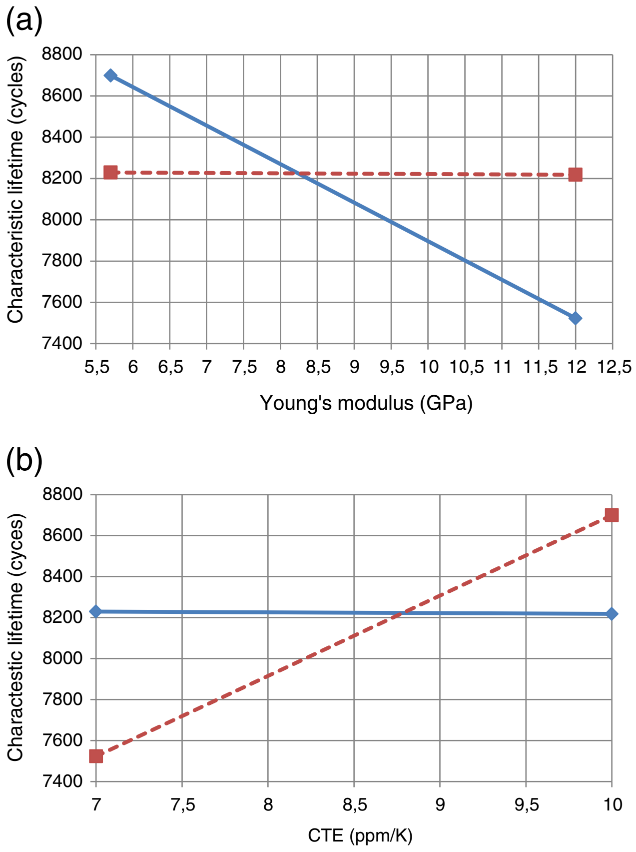

Fig. 6. Graphical analysis of optimum values of Young's modulus between 5.7 and 12 GPa (a) and CTE between 7 and 10 ppm/K (b).

The measurement results are presented in Table 9.

The addition of silica particles into LCP leads to a significant decrease of the LCP Young's modulus in the flow direction. With 10 wt.% filler content, the Young's modulus is similar with or without phenyl functionalization. The minimal Young's modulus is obtained with the smallest silica particle size (sample C).

An 8.3 GPa Young's modulus is expected for a reliable LCP package according to simulations and DoE. Adding silica particles allows the decrease of the Young's modulus in the flow direction as advised by simulations to obtain a maximal lifetime.

Table 7
Optimal results values for CTE and Young's modulus of the LCP.

Parameters	Optimum
	QFN 7 × 7 — 32 leads
Young modulus (GPa)	8.3
CTE (ppm/K)	8.8

Table 8
Samples for mechanical characterization.

Samples	Silica (wt.%)	Specific surface (m^2/g)	Functionalization
A	0	–	–
B	10	170	–
C	10	360	–
D	10	170	Phenyl

Table 9
Young's modulus of the different samples in the flow direction (at room temperature).

Samples	Young's modulus (GPa)
A	14.0
B	11.4
C	10.9
D	11.6

5.2. CTE measurement

A dilatometer (horizontal from 20 °C to 1000 °C) is used for CTE measurements. Parallelepiped specimens (4.5 × 4 × 2 mm) are machined. All measurements are performed in the flow direction.

The CTE is measured as a function of temperature. The results are presented in Table 10.

The addition of 20 nm diameter silica particles into LCP leads to an increase of the CTE in the flow direction (samples B and D). On the contrary adding the smallest 7 nm silica particles into LCP decreases the CTE value (sample C). Whatever the materials, the CTE increases with temperature. A decrease is observed after 100 °C for the LCP alone (sample A) and after 150 °C for the composite with the smallest silica particle size (sample C).

An 8.8 ppm/K CTE is expected for a reliable LCP package according to simulations and DoE. Adding silica particles allows the increase of the CTE in the flow direction as advised by simulations to obtain a maximal lifetime.

5.3. Anisotropy factor

Adding silica particles into the studied precipitated LCP modifies the CTE and Young's modulus in the flow direction in the right way to reach optimum values deduced from simulations and DoE.

In classical isotropic polymer matrix, adding silica induces a decrease of CTE and an increase of Young's modulus. The contrary is observed in the flow direction.

Additional measurements are then performed in the transverse direction. The variation is opposite as in the flow direction: the CTE decreases and the Young's modulus increases (as in classical isotropic polymer).

The anisotropy factor is defined as the ratio of the Young's modulus in the flow direction to the Young's modulus in the transverse direction (measured by Dynamic Mechanical Analysis — DMA). Consequently the anisotropy factor decreases significantly with SiO_2 fillers (see Table 11).

As many commercial polymer, the LCP is loaded with various components such as mica and glass fiber that take the orientation of the injection during molding process increasing the anisotropy. Adding silica changes the preferred orientation and reduces the anisotropy.

The CTE was initially higher in the transverse direction (>8.8 ppm/K) [3]. The change of the anisotropy due to SiO_2 and the balance of properties in the flow and the transverse directions result in the increase of CTE in the flow direction and the decrease in the transverse direction.

Young's modulus was initially smaller in the transverse direction (<8.3 GPa) [3]. These properties in flow and transverse directions

Table 10
CTE of the different samples.

Samples	CTE (10^{-6} ppm/K)			
	50 °C	100 °C	150 °C	200 °C
A	5	7.5	7	3
B	8	11.5	15	14.5
C	3	9	12	10
D	9	12	16.5	20

Table 11
Anisotropy factor (at 50 and 100 °C).

Samples	Anisotropy factor	
	Temperature	
	50 °C	100 °C
A	1.97	2.04
B	1.48	1.50
D	1.51	1.63

counterbalance each other upon silica filler loading around the optimum value deduced from simulations and DoE.

6. Determination of the optimal composition of the LCP composite

According to the DfR results a set of values leading to a maximal lifetime of the QFN package has been determined: (8.3 GPa; 8.8 ppm/K).

Considering the Young's modulus and CTE measurements the expected values seem to be accessible by adding 20 nm phenyl functionalized silica particles. The filler fraction must be still modifying to reach the assessed optimal values leading to the maximal package lifetime.

7. Conclusion

The proposed methodology allows the determination of the optimal mechanical properties in terms of reliability of a material for a given application. In the present study the optimal composition of an LCP composite used as thermoplastic for an electronic package has been determined. The addition of phenyl functionalized 20 nm silica particles enables to reach mechanical properties close to the simulated optimal values for Young's Modulus and CTE leading to a maximal lifetime of the package.

This methodology allows to considerably reduce the number of experimental studies that are very time consuming and to develop reliable and dedicated materials with optimal mechanical properties for a targeted application.

QFN packages based on LCP with phenyl functionalized 20 nm silica particles (10 wt.%) will be made and tested in the near future.

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