RELIABILITY-BASED OPTIMIZATION USING GENETIC ALGORITHMS TO DETERMINE THE AREA FOR BONDING WHERE COPPER METAL THIN FILMS ARE DEPOSITED ON A FLAT SURFACE POLYMER POLYPROPYLENE

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Abstract. *In this study it is present a methodology for reliability-based optimization systems where copper metal thin films are deposited on a flat surface polymer polypropylene. The input data of this metal-polymer joint is the normal stress required to detach the copper film from the substrate of polypropylene through different forces and interface areas, obtained from the uniaxial tensile test, ASTM D5179-02. The knowledge of the maximum force that supports the interface, the methodology RBDO (Reliability Based Design Optimization) was implemented to find the smallest diameter of the circular area sandwiched necessary to ensure different levels of reliability, thus, minimizing the cost (less metal area film). Considering the minimum diameter or area of film deposited, the analysis aims also the minimum metal quantity deposited as a cost criterion. The reliability is treated as another input data, specified by the user and it acts as an additional constraint to the problem. As an optimization methodology, it is used the global search method, genetic algorithms, due to its favorable behavior to nonlinear functions.*

Keywords*: uncertainty, optimization, reliability based design optimization, polymer.*

1. INTRODUCTION

The desire to obtain optimized conditions, achieving lower cost, higher efficiency and better performance has always been a big goal of manufacturing engineering. In this work we use the global search method, genetic algorithms (GA) to obtain optimal values to minimize a circular interfacial area to refine the duet: cost versus film strength under particular stress, respecting the reliability indexes.

The metallization of polymers has been applied in several areas, either in the electronics industry by means of printed circuit boards, the food industry using metalized food packaging and even in biomechanics to improve the surface wear of prosthetic components with polymer. For a successful use of metalized polymer among its many applications, it is necessary to control the quality of the adhesion of metal film on polymer substrate. It is known that temperature affects significantly the size and mechanical strength of polymers; therefore, control this variable is an indication of performance in the metallization process. As the effectiveness of the interface in the control of adhesion of the materials, ensuring that there are no problems like lack of anchoring, such as peeling, formation of micro cracks and wear of the thin film.

The mechanisms of adhesion shall ensure the function of the composite material and should also define the more appropriate pair of metal-polymer material, making a cost-benefit analysis or energy expenditure versus property. There are several ways to determine the interface strength, qualitatively or quantitatively. The last one refers it self as the data for the joint design that could correlate a normal stress or a tangential one to a failure criteria; thus, defining values to use in the selection of such composite materials.

There are several papers about metallization of polymers, where adhesion has been evaluated, and the interface conditions modified in order to assess their influence on the joint [Yang et al., (2005); Kondoh, (2000); George et al., (2005), Mackova, (2008); Wolf, (1999)]. The technique of surface cleaning by spraying ions onto the sample was reported by Fujinami, (1998), where the influence of pretreatment of titanium films on polymer substrates was studied. The results showed that the change of morphology of polymer can improve the adhesion of the composite. Other techniques are also used to modificate the surface, such as buckling, etching and plasma immersion [Pinto, (1999)], but all these methods have a common goal, the changing of adhesion. Another important factor is the low surface free energy for the polyolefins such as polypropylene, which leads the tendency of a weak chemical bond in the film-substrate interface [Novak e Florian, (1999)].

2. EXPERIMENTAL DATA-DETAILS

Thermoplastic polymers were mould injected into specimen following the dimensions: 3.2 x 12.5 x 25.0 mm. The roughness of injection molding is similar to the samples injected. The metallization on polymer was made through copper evaporation by an electron beam irradiation at a vacuum chamber (2.3x10-6 kPa). The samples were recovered by the copper vapor until the desired thickness, around 0.5 µm.

The preparation of polymer composites coated metallic thin film is the first step of the present work, the second step follows with the detachment of thin copper film of polypropylene polymer. A tensile testing machine with a load cell of 1000 N capacity was used to measure the normal force of adhesion. The test follows the recommendations of ASTM D 5179-01 (2008), with a pull-off speed of 2 mm/min at an ambient temperature of 23°C, relative humidity of 50% and pressure between 86 and 106 kPa. The test results will be the maximum pull-off strength of the film and the area where the metal film would be removed, obtaining a normal force and a normal area to detach the joint.

The pull-off test measures the stress necessary do delaminate the film of a substrate, such value is the normal ultimate tensile stress, which is largely used as failure criteria for these composites (Silva et al., (2007)).

3. RBDO (RELIABILITY BASED DESIGN OPTIMIZATION)

The RBDO is an optimization process which aims the minimization/maximization of cost function and satisfies reliability constraints as initial conditions. For this reason, it is necessary perform probability analysis during the optimization process. Besides, the design variables can be probabilistic parameters so that the optimization task became more complex.

The simpler and common formulation in the RBDO implementation is separated in two levels:

(a) An outer loop to perform the optimization, where the design variables are taken into account;

(b) An inner loop to perform the reliability analysis.

Generally speaking, an optimization model can be defined in the following way: Minimize (or Maximize) a cost function subjected to constraints. In a mathematical notation:

$$Minimize\ f(vp;\ p) \tag{1}$$

Subjected to

$$\begin{aligned} &gi(vh;\ p) = 0 && i = 1 ... nr \\ &gi(vh;\ p) < 0 && i = nr + 1 ... nr \\ &vhl < vh < vhu && i = 1 ... nv \end{aligned} \tag{2}$$

where vh are the design variables, p are the constant parameters of the problem, g_i is the i-th model constraint, vhl and vhu are respectively the lower and upper limit for the design variables. The deterministic optimization does not consider uncertainties in the design variables. Using the RBDO methodology, the constraints in the deterministic formulation are changed by probabilistic constraints. By the probability theory, it is well-known that the reliability index can be written as function of the failure probability as:

$$\beta = -\Phi(P_f(vp;p)) \tag{3}$$

where Φ is the cumulative probability function.

3. GENETIC ALGORITHMS

Genetic Algorithms (GA) are optimization techniques based on the Darwin's Theory of evolution and survival of the fittest. The Darwin's Theory of Natural Selection (1859) *apud* Goldberg, (1989) says that "… any being, if it varies slightly in any manner profitable to itself, will have better chance of surviving…". GA simulates the evolutionary process numerically. They represent the parameters in a given problem by encoding them into a string. As in genetics, genes are constituted by chromosomes. Similarly, in simple GA, encoded strings are composed of bits. A string of bits can be decoded to the respective problem parameter value and the total evaluation of the string of bits for and individual may be weighted following some fitness function representing the phenotype to that string of bits.

A simple genetic algorithm consists of three basic operations (Holland, (1975)), these being reproduction, crossover and mutation. The algorithm begins with a population of individuals each of them representing a possible solution of the problem. The individuals, as in nature, perform the three basic operations and evolve in generations where the Darwin's Theory prevails, or in other words, a population of individuals more adapted emerges as natural selection.

The floating point Coded Genetic Algorithms assumes real values to each variable. The main differences in this method are found on the crossover operator. There are several methods to deal with the floating point Coded Genetic Algorithms crossover such as flat crossover, simple crossover, arithmetical crossover, Wright's crossover, linear BGA crossover, etc. In this paper the BLX-α was used because it uses an initial exploration of the parameters field followed by an exploitation phase to improve resolution. It may be described by:

$$\Delta = max[b_i(k), b_{i+1}(k)] - min[b_i(k), b_{i+1}(k)] \tag{4}$$
$$b(k) = random\{min[b_i(k), b_{i+1}(k)] - \alpha\Delta,\ max[b_i(k), b_{i+1}(k)] + \alpha\Delta\}$$

where, i and $i+1$ are referred to two parents' chromosomes, α means a decreasing exploration parameter and random means a random number in the respective interval. Figure 2 summarizes the main steps followed by a Floating Point Coded basic Genetic Algorithm to maximize functions.

As indicated by Fig. 1, the algorithm starts generating a random set of individual that will form the population. In the following, individual are selected and picked on pairs according its fitness (objective function). This is accomplished by a probabilistic raffle called roulette wheel. At this point crossover will occurs, mixing chromosomes from two individual generating two offspring with characteristics inherited from its parents. The reproduction will be promising with a probability of 'Pc'. At last, from the offspring population, some chromosomes of some individual will suffer mutation under a probabilistic rate of 'Pm' usually set as a low value (1% or less) as found in nature. Then, eventually, some best individual belonging to the parent set will bypass the natural selection and will be introduced in the offspring set through an elitism procedure and exchanged by the less fitted offspring. This procedure assures that best solutions are hold and not lost in the probabilistic selection. The generations will succeed until a convergence criterion being reached. In this paper the stopping criteria is the diversity on the population set evaluated by the standard deviation of the objective function (fitness).

Step i) Initialize Time $t=0$, Initialize Population size: "*m*", mutation probability: "*Pm*", crossover probability: "*Pc*", number of individual chromosomes: "*nc*", allowed limits for each chromosome: "*Pmax(nc), Pmin(nc)*".
Step ii) Generate Initial Population: $B_0 = (b_{1,0}, b_{2,0}, \ldots, b_{m,0})$
Step iii) While Stopping Condition is not fulfilled
Step iii-1) "Proportional Selection"
Loop $i=1$ to m
$x=random\ (0,1)$
$k=1$
While $k<m$ and $x< \sum_{j=1}^{k} f(b_{j,t}) / \sum_{j=1}^{m} f(b_{j,t})$
$k=k+1$
$b_{i,t+1} = b_{k,t}$
End While
End Loop
Step iii-2) "One Point Crossover"
Loop $i=1$ to $m-1$ step 2
If random $(0,1)<Pc$ then
$\alpha = 0.5$
$\Delta = max[b_{i,t}(k), b_{i+1,t}(k)] - min[b_{i,t}(k), b_{i+1,t}(k)]$
$b_{i,t+1}(k) = random\{min[b_{i,t}(k), b_{i+1,t}(k)] - \alpha\Delta,\ max[b_{i,t}(k), b_{i+1,t}(k)] + \alpha\Delta\}$
$b_{i+1,t+1}(k) = random\{min[b_{i,t}(k), b_{i+1,t}(k)] - \alpha\Delta,\ max[b_{i,t}(k), b_{i+1,t}(k)] + \alpha\Delta\}$
End If
End Loop
Step iii-3) "Offspring Mutation"
Loop $i=1$ to m
If random $(0,1)<Pm$ then
$k=random\ (0,1)*nc$

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    b_{i,t+1}(k) = random{P_max(k), P_min(k)}
  End if
 End Loop
End Loop
```

Figure 1. Pseudo-Code for the floating point genetic algorithm codification.

4. FORM : FIRST ORDER RELIABILITY ANALYSIS

A mathematical expression for the failure of a system may be stated in the following way:

$$M(x) = g(X_1, X_2, ..., X_n) \leq 0 \tag{5}$$

where means the safety margin and are the vector of n probabilistic variable that affects the material strength. means failure and means that the system is in the safe domain. The failure probability can be calculated using the jointly probability density function as (Melchers, (2001)):

$$P_f = \iint \cdots \int_D f_x(X_1, X_2, ..., X_n) dX_1 dX_2 ... dX_3 \tag{6}$$

where D is the domain where $M \leq 0$. Taking into consideration a truss structure, where the failure function is defined by the stress σ_i in a member related to the allowed stress $\sigma_{\lim}$, the safety margin (limit state function) is written as:

$$M = 1 - \sigma_i / \sigma_{\lim} \tag{7}$$

This methodology can be used to compression stresses, displacements or any other function that indicates undesirable condition violations. Integration of Eq. (6) is difficult. Besides, sometimes statistical parameters of $f_x(\mathbf{X})$ are not known *a priori*. For this reason, it is usual use the first and the second moments (mean value and standard value) to calculate the reliability index β of the safety margin *M*. The known FORM (*First Order Second Moment*) uses an approximation of the limit state function in the vicinity of the design point in order to evaluate the β index. Besides, the FORM allows calculating the reliability index independent of the expression used as safety margin. For non-correlated variables, the random variables X_i can be transformed into standard non-correlated variables U_i taking:

$$U_i = \Phi^{-1}\left[F_{x_i}(X_i)\right] \tag{8}$$

where $F_{x_i}(X_i)$ and Φ are the cumulative distribution function and the Standard cumulative distribution function for variable X_i, respectively. In this way the safety margin in the real space can be transformed to the non-correlated standard space U :

$$H(\mathbf{U}) = M(\mathbf{X}) \tag{9}$$

A first order approximation of the limit state function on point $\mathbf{U}^*$ can be drawn and the gradient descent method can be used to find the smallest distance from approximated limit state function $H(\mathbf{U}) = 0$ to the origin of the non-correlated standard space $\mathbf{U}$. The $\mathbf{U}^*$ point is called design point and the reliability index β can be calculated as the Euclidian distance to the origin of the non-correlated standard normal space as:

$$\beta = \min(\mathbf{U}^{*T} \cdot \mathbf{U}^*)^{1/2} \tag{10}$$

In order to solve this problem Eq. (11) it is used an iterative solution proposed by Rackwitz – Fiessler (1978) *apud* Haldar e Mahadevan, (1999), which can be described as:

$$U^*_{i\,k+1} = \left[\nabla M(U^*_{i\,k})^t U^*_{i\,k} - M(U^*_{i\,k})\right]\nabla M(U^*_{i\,k}) / \left|\nabla M(U^*_{i\,k})\right|^2 \tag{11}$$

where ∇M is the limit state function gradient (safety margin), U is the vector of probabilistic variables in the non-correlated normal space.

In Eq. (11) all the variables in the real space are considered non-correlated. If there exist any correlation it may be used a Cholesky decomposition of the covariance matrix in order to transform from real space to non-correlated Normal space (Haldar e Mahadevan, (1999)).

4. RESULTS

This work aimed to reduce the bonding area. Considering a circular area, the design parameter was the diameter, given the constraints of system reliability (β = 2, β = 2,5 e β = 3,0). The load varied from 1 to 1000 (N), and the diameters 0.1 to 300 mm. The uncertainties of the model were obtained from experimental data, it was found that the average area required is correlated with the applied force, the factor covariance is 0.33 and the distribution is lognormal.

In this case, for the design variable, the algorithm itself is responsible for ensuring non-violation of the upper and lower limits, however, if occurs violation on the limit of reliability index, it is applied a penalty in the objective function.

Specifically, it is shown in the following Equation $penalty = C[1 + H(g_i^r)]$, where H is a step function (whose value is zero if $g_i^r \leq 0$ or the value of g_i^r, when $g_i^r > 0 > 0$ and C is a penalty constant (in this work taken to be C = 100).

In this work, GA was used with 20 generations consisting of 50 individuals each, with a crossover fraction of 0.8, a mutation fraction of 0.5 and an elitism of 2 (More information about these parameters can be found in Goldberg, (1989)).

In all the cases studied, the optimization algorithm terminated when it reached the number of individuals and generations specified by the input data of the optimization algorithm.

$$Min(FO) = penalty + (area) \tag{12}$$

In Figure 2 it is possible to verify the behavior of the curve of the diameters required for each force and for each of the three indices used as a reliability constraint.

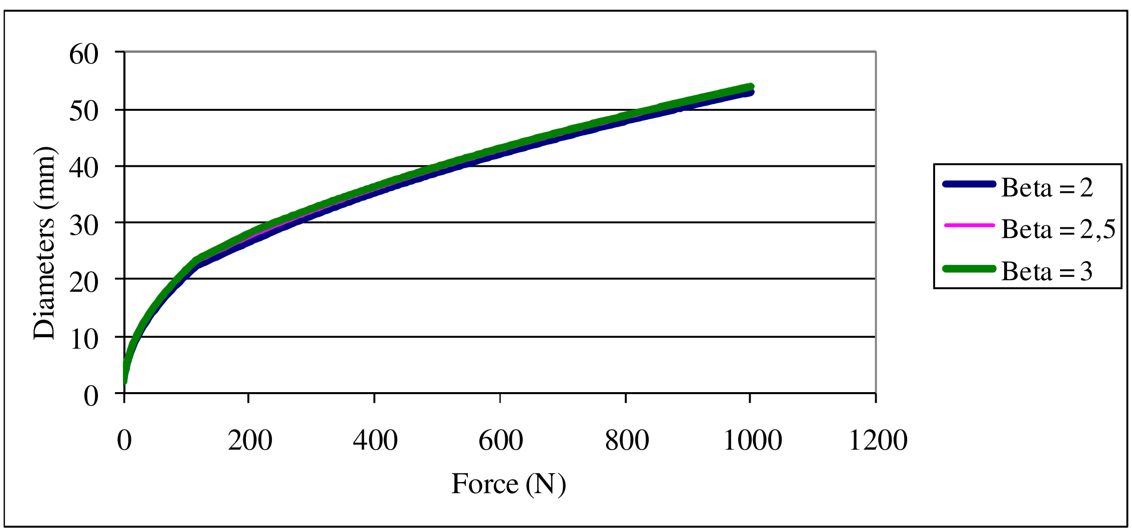

Figure 2. Values obtained with the reliability-based optimization for different forces and reliability

Based on this figure, the proximity of the lines shows that small variations in diameter can lead to substantial improvements or worsening in relation to the reliability of the system, this is due to the value of the covariance factor, this occurs because this value is considered high.

5. CONCLUSIONS

This From the results it was possible to show that the use of reliability-based optimization is applied to identify the optimum parameters for bonded surfaces, minimizing the area (hence cost) and considering the probability of failure.

The index of reliability allows to achieve the required values for the design variables in a consistent manner, avoiding oversize of systems, consequently avoiding wastage of raw material.

The employed methodology is robust enough and allows the imposition of more restrictions. It could be used in several similar cases

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