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RESEARCH ARTICLE

MICROWAVE ELLIPSOMETRY CHARACTERIZATION OF ISOTROPIC MATERIALS USING SIMULATED ANNEALING COMBINED WITH LEVENBERG-MARQUARDT ALGORITHM.

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Abstract

The characterization of thick materials using microwave ellipsometry is known as non destructive technic. New microwave Ellipsometry has been developed and tested at different frequencies: in the 24-40 GHz frequency band and at 10 GHz. Several materials were characterized through this device using Levenberg-Marquardt optimization routine. Complex objective function with several local minima has been to be solved. Many recent works have shown that this routine has been very efficient in finding local minimum, but not for global minimum unless using some tricks. In this paper, we have combined two algorithms, namely simulated annealing and Levenberg-Marquardt algorithms, in order to enhance the characterization technic in finding the global optimum. Simulations were performed and concluded that the combined algorithm is more efficient than any of its basic algorithms. Experimental results on PTFE sample considering Cauchy dispersion model validated the simulation assumption.

Introduction:-

The characterization of materials has always been a preoccupation for manufacturers in the development of their various products. Some technics damage the product to be characterized at the end of the process. Others do not damage it and are called non-destructive technics [1]; they are usually contact free.

Characterization by microwave polarimetry, also called microwave ellipsometry, falls into this second category. It was first an optical method [2], and then has been extended to the microwave domain. Several configurations related to different technics exist. However, any configuration has basic elements which are polarizer, compensator and analyzer [1].

Generally, ellipsometry technics make it possible to determine the properties of samples (thicknesses of refractive index n and extinction index k) via intermediate parameters called ellipsometric parameters (ψ, δ) [3]. The technic we are interested in is made up with a rectangular waveguide as a polarizer and three detectors as analyzers. This type of ellipsometer has been the subject of several studies in the band 24-40 GHz. This ellipsometer has made it possible to characterize various types of samples from various isotropic or anisotropic materials. Examples include the characterization of composite materials [4], natural wood and agglomerated wood [5] and Teflon [6, 7]. This device was also developed for 10 GHz operation and has been used to characterize anisotropy [8], and to characterize wood palmyra samples [9]. The extraction of the parameters of the samples is done with the Levenberg-

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Marquardt optimization algorithm. Unfortunately this algorithm is sensitive to local minima. In this work, we deal with a comparative study between the Levenberg-Marquardt algorithm, simulated annealing, and a combination of both algorithms. Finaly, we will present the experimental results done on polytetrafluoroethylene (PTFE) sample. PTFE is known as non-absorbent (k close to 0), its relative permittivity n=2.1, its loss tangent is 0.0003, and its service temperature is relatively also high (~250±1°C) [10, 11].

Material And Method:-

Presentation of the microwave ellipsometer:-

The device is shown in Figure 1. It consists of a transmitting part and a receiving part. The incident wave is produced by a Vecterial Network Analyser in the frequency range of 24 to 24 GHz. The generated electromagnetic wave goes through a rectangular waveguide that polarizes the electric field E parallel to the small side, so that only the fundamental mode TE10 propagates. The wave is collimated by a horn carrying a Fresnel lens, afterward it propagates in free space before crossing the sample placed in a plane inclined at an angle φ0 with respect to the direction of propagation. The interaction between the wave and the electromagnetic characteristics of the sample under test modifies the polarization of the TEM wave which, in general, becomes elliptical. A cornet-Fresnel lens assembly, identical to that of the transmitting part, receives the emergent elliptical polarization. It continues its course through a circular waveguide in the receiving part. It reaches a short-circuit positioned at the connection of the three rectangular waveguides, placed in the transverse plane and directed at 120° from each other. Thus, the incident and reflected waves at the short-circuit mix up to form a stationary wave that propagates through the three receiver branches. Each branch consists of a rectangular waveguide, an isolator and a detector microwave all operating at 10 GHz. Therefore, each detector receives an electromagnetic power corresponding to the radius of the ellipse where it is placed (Figure 1). The set up of this free-space experimental bench is based on preliminary works described in [12], except the fact that the Gunn source is replaced by a Vector Network Analyzer (VNA).

Figure 1 shows both fixed emitting and receiving parts aligned for transmission measurements. The sample is placed between the emitting and receiving parts, and is inclined with respect to the direction of propagation to have oblique incidence where φ is the incidence angle. The sample is mounted on a revolving plate actuated by a stepper motor. When rotating, the position of the sample is given by θ, (called the angular position or azimuth θ), which is measured from the direction of the emitted linear polarization [7, 13].

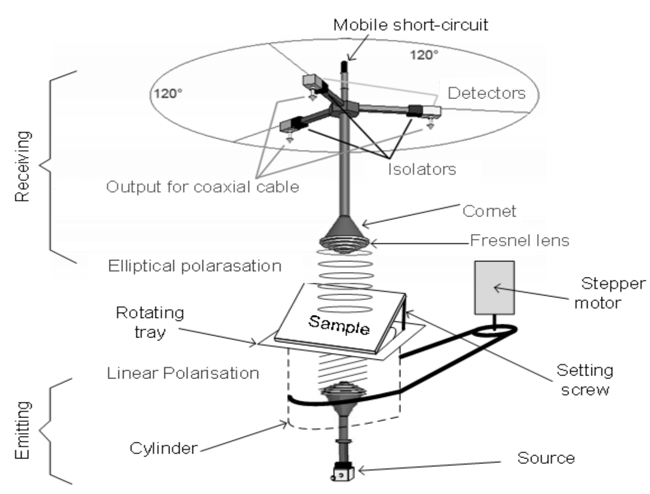

Figure 1:-Polar bench configuration.

Measurement principles:-

When an isotropic sample is excited with an electromagnetic wave whose direction of propagation is indicated by an angle φ0 with respect to the normal of its surface, there will be multiple reflections and transmissions as shown in figure 3. Thus, waves meet two interfaces:

1. air-sample;
2. sample-air.

Considering n_0 the optical index of the air and n_1 the optical index of the sample, then:
$n_0 = 1$
$n_1 = n + jk$
where n and k are respectively the refractive index and extinction coefficient of the isotropic sample.
Also, n and k can be expressed using Cauchy dispersion law as:
$n = A + \frac{B}{\lambda^2}$
$k = D\lambda + C\lambda^2$
where A, B, D and E are Cauchy dispersion parameters of the sample, λ is the wavelength.

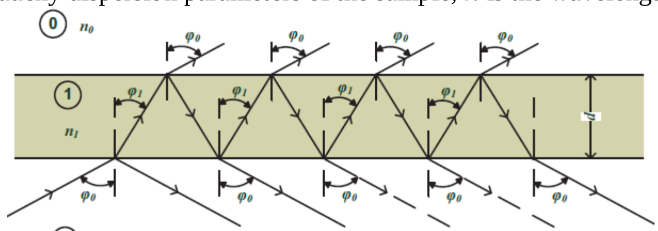

Figure 2:-Multiple reflections and transmissions interaction.

The reference [13] give in detail the different equations that lead to equation (5) that relates ellipsometric parameters ψ and δ and the parameters of the sample:
$\rho(\Psi, \delta) = \frac{R_P}{R_S}$

where R_P and R_S are respectively the total transmission coefficients of the structure along the parallel planes and transverse to the plane of incidence.
The ellipsometric parameters depend on the optical indices, the thickness, the angle of incidence and the frequency f, but they do not depend on the azimuth θ. Moreover, the measurement of the three electromagnetic intensities is obtained through the ellipsometric microwave bench that makes it possible to determine these ellipsometric parameters through the following relation [7]:
$\gamma = \alpha + \theta$
and
$\tan(2\gamma) = \frac{\tan(\Psi)\tan(\theta)}{tan^2(\Psi) - tan^2(\theta)}\cos(\delta)$

The frequency f, the angular position of the sample or azimuth θ and the angle of incidence φ0 are the measurement conditions; the angles α and γ are called rotations.
To better describe the different angles involved in the wave-matter interaction, we define three coordinate systems (Figure 3):
- (O, X, Y) bound to the laboratory;
- (O, P, S) bound to the sample;
- (O, X ', Y') bound to the ellipse.

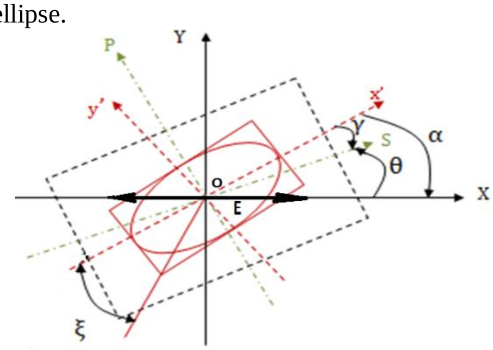

Figure 3: Description of the interaction

Solving the inverse problem:-

We deal with a global minimization problem. It can be formulated as a pair (S,F), where $S \in \mathbb{R}^n$ is a bounded set on $\mathbb{R}^n$ and $F(S) \in \mathbb{R}$ an n-dimensional real-valued function. The problem now is to find a point S_opt so that $F(S\_opt)$ is globally minimal on S. In real case, the objective function f is required to meet the goal $F(S\_opt) < \varepsilon$. From the equation (5), the objective function can be defined as:

$$\mathrm{F}(\Psi, \delta, \theta) = \tan(2\gamma) - \frac{\tan(\Psi)\tan(\theta)}{tan^2(\Psi) - tan^2(\theta)}\cos(\delta)$$

where Ψ and δ are the ellipsometric parameters, both depending on the refraction index n**,** the extinction coefficient k**,** the thickness of d, the incidence angle φ**,** and the frequency f [7].

In this equation, the rotation γ is measured through the ellipsometric bench, and the conditions of the measurement, which are θ, φ and f, are known. The unknown variables of in the objective function are n and k. We define S as the set of the properties of the sample to be found so that S=[n,k] meeting the goal:

$$\mathrm{F}(\Psi, \delta, \theta) \leq \varepsilon$$

Three numerical methods, which are namely the Levenberg-Marquartd optimization algorithm, simulated annealing and the combination of both of them, are experienced.

Levenberg-Marquardt algorithm:-

Developed in the early 1960's, the Levenberg-Marquardt algorithm is a fitting method to solve nonlinear least squares problems. The main disadvantage of this algorithm is the fact that you should know the close nearby solution area. Beacause it converges to different local minima depending upon values of the initial guess, the measurement noise, and the algorithmic parameters [14].

Simulated annealing:-

Simulated annealing (SA) is a Metaheuristic search technics for solving optimization of many-variable. It derives its name from an analogy to the cooling of heated metals at melting temperature. It models the physical process of heating a material and then slowly lowering the temperature by slow stages until the system freezes and no further changes occur.

This method can always get out of a local optimum at nonzero temperature [15]. Indeed, a given state with energy E1 is compared to another state with energy E2. The new state is obtained by moving one of the particles of the former to another location by a small displacement. If $\Delta E = E1 - E2 \leq 0$**,** the new state is accepted because the move brings the system in a state of lower energy; i.e. transitions from the current state to a new state with lower energy are always accepted. But if $\Delta E = E1 - E2 \geq 0$, the is accepted with probability $\exp(-\Delta E/\mathrm{kT})$, k is the Boltzmann constant and T the temperature of the heat bath [16, 17]. This means that some moves to higher energy are accepted helping the system not get stuck on a local minimum.

The algorithm parameters are:-

1. Initial temperature : T0 ;
2. Maximum iteration : imax ;
3. Geometrical cooling coefficient: α; it is a constant between 0 and 1; to have as low decrease of temperature, it is better to set α closer to 1 [18].

The simulated annealing algorithm performs a random walk in the configurations space, starting from a random initial state. The temperature is decreased only when the system is in thermal equilibrium at the current temperature. In the algorithm given in figure 4, X0 is the initial guess vector consisted of n and k. The energy is the objective function F given in equation 6. The variables m_s and m_fs refer to current optimum guess and objective function.

Simulated annealing – Levenberg-Marquardt algorithm:-

The benefit of the combination of simulated annealing and Levenberg-Marquardt algorithm is to develop an algorithm which is more efficient than both of them. First, the simulated annealing finds initial guess in the nearby of the global optimum of the objective function. Then the Levenberg-Marquardt is performed to determine its accurate value.

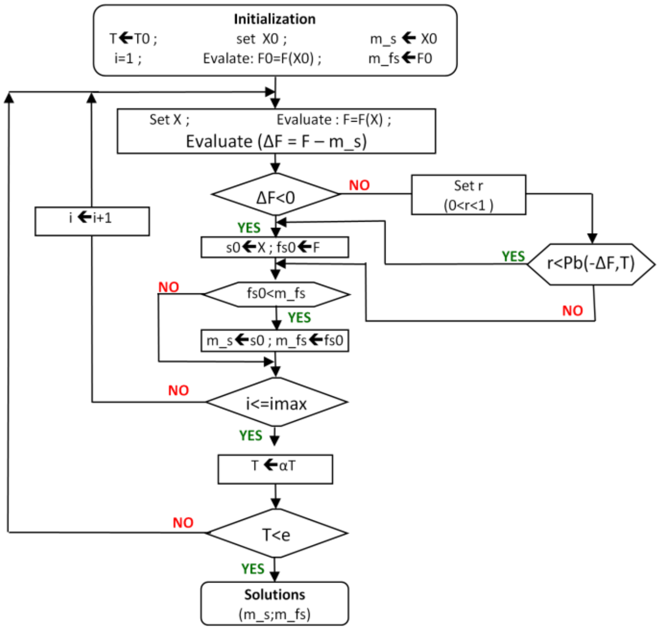

Figure 4:-Full simulated annealing algorithm.

Results and Discussion:-

Simulations:-

First, we computed several simulations in the same time with the three algorithms in order to compare their efficiency. The comparison is based on the accuracy of the values of the dispersion parameters obtained by each algorithm. Moreover, the simulations help us check the best setup (coefficient α and initial temperature T0) of the simulated annealing.

To do so, we consider some examples of theoretical values of the dispersion parameters A, B, D and E to be determined:-

1. thickness: d= 1 mm;
2. Cauchy dispersion parameters : $A = 1.5$; $B = 6.10^{-5}$; $D = 10^{-3}$; $E = 8.10^{-8}$;
3. Experimental conditions: $= [0°: 30°: 360°]$; $\varphi = 30°$; $f = 30$ GHz.
4.

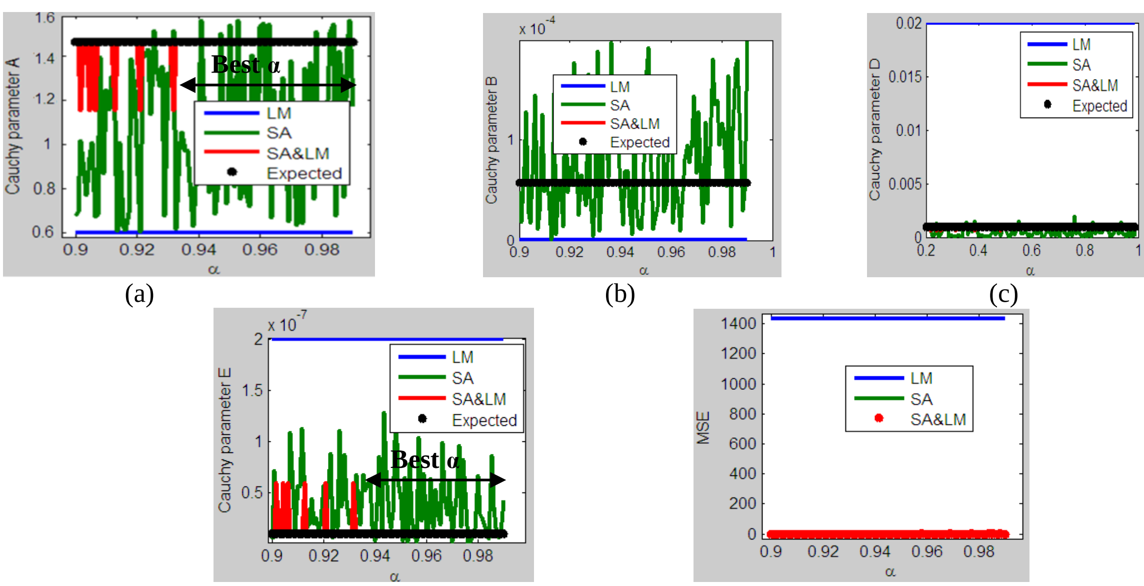

Figure 5:-Influence of the parameter α (T_0=10;imax=100):-

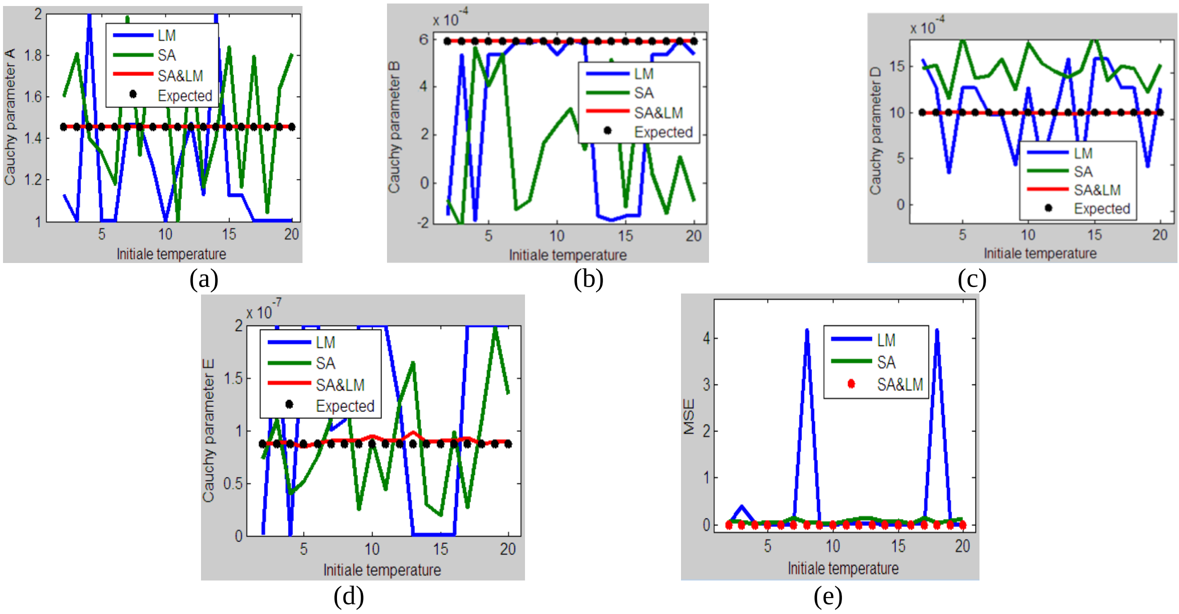

Figure 6:-Influence of the initial temperature (α=0.99; imax=100).

The results of the simulations given in the figures 5 and 6 show that, in any case of the four parameters, the combined simulated annealing – Levenberg-Marquardt algorithm (SA&LM) fit the best. As said earlier, the best setup of the simulated annealing is met with α close to 1, but there is no big issue with the initial temperature when its value is greater than 15.

Experimental results:-

To validate the simulation result which suppose that the combined algorithm is more efficient than the two other separately, we tested a PTFE sample whose thickness is 1 mm. The test was performed under the following conditions :

- $\theta = [0°{:}30°{:}360°]$;
- $\varphi = 30°$;
- $f = 30\ GHz$.

The simulated annealing is computed for α=0.99, initial temperature T0=10 and itmax=100.

The results of the characterization are presented in the table 1 and the fitting curves in the figure 7.

Table 1:-Values of optics parameters extracted with the three methods.

	Levenberg-Marquardt (LM)	**Simulated annealing (SA)**	**SA&LM**
A	1.0000	1.0757	**1.0131**
B (10^-3)	0.0000	0.8956	**0.6854**
D	0.0000	0.0059	**0.0013**
E (10^-6)	0.0000	0.0433	**0.1037**
n	**1.2020**	**1.7086**	**1.4974**
k	**$1.0794\text{x}10^{-07}$**	**0.5540**	**0.0017**

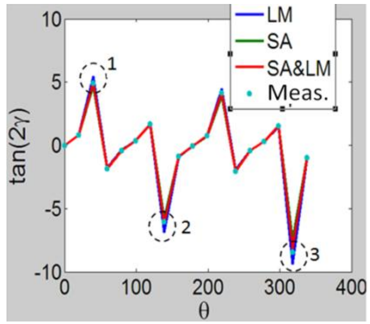

Figure 7:-Experimental **c**haracterization curves for a PTFE sample (d=1 mm).

The table 1 shows that the values of the dispersion parameters given by the combined algorithm gives refraction index and extinction coefficient too close to their known values than those given by the two other algorithms separately. This confirm that the simulated annealing – The Levenberg-Marquardt algorithm is more efficient than its basic algorithms. However, the three fitting curves a very close except at the three points (1, 2 and 3) indicated in the figure 7. This means that the combined algorithm is very sensitive.

Conclusion:-

This paper introduced the efficiency study of the combination of the simulated annealing and the Levenberg-Marquardt optimization routines applied to microwave measurement. It is the first study of using this algorithm for measurement done through the three-detector microwave ellipsometer. The robustness of this algorithm has been demonstrated in comparison with basic simulated annealing and Levenberg-Marquardt algorithms. Considering isotropic material described by Cauchy dispersion model, the convergence of the SA algorithm was most efficient with a linear decrease of the temperature by a coefficient $\alpha = 0.99$, where initial temperature is greater than 10 and the maximum iteration number is equal to1000. Simulations results and experimental results on PTFE sample have led to this conclusion.

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