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60 Abstract : The design efficiency of two different optimization techniques of designing multilayer optical thin film devices is compared. Ten different devices of varying complexities are chosen as design examples for the comparison. The design refinement efficiency and the design parameter characteristics of all the sample designs obtained with the two techniques are compared. The results of the comparison demonstrate that the new method of design developed using damped least squares technique with indirect derivatives give superior and efficient designs compared to the method developed with direct derivatives.

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1. INTRODUCTION

Optical multilayer thin film devices with their characreristic properties like very high reflection, very low absorption, very high throughput energy etc, play a vital role in many front line research activities like laser fusion, laser isotope separation, Optical communications, use of synchrotron radiation, use of neutron beams, solar energy and space research for the control of electromagnetic radiation ranging from x-ray to sub-millimeter spectral region. Some examples of such thin film devices are anti reflection (A.R) coatings, high reflection (H.R) dielectric mirrors, output couplers, Fabry-Perot Mirrors, beam reflectors, beam splitters, band pass filters, edge filters, polarizers, optical wavelength multiplexer and demultiplexer etc.

The theory and principles of design and fabrication of multilayer thin film devices are very well known[1-6] but the development of these devices for the above modern applications[7-12] requires complex and specialized design and fabrication techniques the details of which are not available completely in the literature. R&D facilities are being set up in the Spectroscopy Division to develop both thin film design and thin film fabrication technologies indigenously. Two new optimization methods[13,14] were developed to design complex thin film devices according to the required specifications. These methods have certain advantages and disadvantages compared to one another. The design refinement and design parameter characteristics of different thin film devices obtained with these two optimization techniques are compared in this report.

2. THIN FILM DESIGN TECHNOLOGY

To design simple thin film devices like single layer single band A.R.Coating, multilayer single band H.R.Coatings and narrow band filters is not difficult and such designs are very well described in the text books[1-6]. But designing complex thin film devices like two band A.R. and H.R.coatings, broad band A.R. and H.R.coatings, broad band beam splitter, broad band F.P.mirror, edge filters etc. is a difficult task and cannot be done in a straight forward way because the problem involves in solving a large number of highly nonlinear equations with very few variables and with many constraints. During the last two decades or so thin film designers proposed[11-19] elaborate and complex methods to solve the design problems using different algorithms and techniques. Most of the design methods reported so far are based mainly on three basic approaches[4-6] namely i)Graphical methods, ii)Analytical methods and iii) Digital methods. Out of all these methods Digital methods are more power full compared to other methods in giving the required designs with complex properties. Digital design techniques are again divided into two types as optimization methods and synthesis methods. Optimization methods or Refinement methods are relatively easy to develop and so they are being used extensively for thin film design.

3. DIGITAL OPTIMIZATION METHODS OF THIN FILM DESIGN

In optimization methods[13-20] a rough design whose spectral characteristic matches very approximately with the required characteristic is taken as initial design and its performance is improved or refined by changing the film thicknesses in an iterative way by employing different optimization techniques like normal least squares method, damped least squares method with direct derivatives, damped least squares method with indirect derivatives, steepest descent method, Adoptive Random Search method, Golden Section method etc. Since thin film design problem is highly non linear some optimization methods perform better than others in minimizing the corresponding merit function and hence in getting the required design efficiently[22]. In the case of Damped Least Squares Optimization methods the design problem mainly consists in minimizing a defect function ψ given by

$$\psi = \sum_{i=1}^{n} [\Delta R_{\lambda i} \cdot W_i]^2$$

which is the sum of squares of reflection differences $\Delta R_{\lambda i}$ between the desired and the initial designs multiplied by suitable weightage factors W_i at the iven n wavelength points. The defect function of the initial design is evaluated first and if it is more than the specified value, the method solves a set of equations to minimize ψ by changing the film thicknesses. The new film thicknesses are incorporated in the initial design giving rise to an improved design. The extent of design refinement and the efficiency of the method mainly depend on the optimization technique used and also on the magnitude of the initial defect function. In general the drawback of a least squares optimization method is that it gives good improved designs only if the defect function ψ of the initial starting design is relatively small. With such limitation an optimization method using damped least squares technique with direct derivatives was developed earlier[13] which is referred as "old design method" or "old design technique"in the following pages. The above limitation was resolved in two ways i) by using an additional matching or limited scan[17] stage before optimization or ii) by using a new optimization technique[14] with indirect derivatives. The later method is referred as " new design method" or "new design technique" in this report. The design refinement efficiency and the design parameter characteristics of different optical multilayer thin film devices obtained with old and new design methods are compared in detail as follows.

4. THIN FILM DESIGN PROCEDURE USING THE OLD AND NEW DESIGN METHODS

The procedure of designing a thin film device using the old method consists of three stages whereas the design procedure takes only two stages using the new method as shown in Fig.1. As can be seen in Fig.1(a), for designing a 15 layer edge filter using the old method a rough simple design *A* (quarter wave stack) whose spectral characteristic matches very approximately with the required characteristic is taken as starting design. Since the old method requires an initial design with relatively small ψ for efficient refinement , the ψ of the starting design is reduced first to a limited extent by using a matching or scanning technique in stage *B*. The design thus obtained is improved further in an iterative way by employing the old optimization method in stage *C* to get the final design. This procedure unusually takes a long computer time and in some cases it fails to give the required minimum defect function ψ in stage *B*. For such cases the second design procedure (Fig.2(b)) was successfully applied to get the required design efficiently wherein the initial quarter wave stack is directly taken and improved using the new optimization method.

5. OLD AND NEW OPTIMIZATION METHODS OF DESIGNING THIN FILM DEVICES

The same optimization technique of Damped Least Squares is used in both the old and new design methods. The main difference between them is in the method employed for computing the partial reflection derivatives with respect to film thicknesses needed in the optimization calculations. For a multilayer optical thin film device of *m* films its reflectance R_{λ_i} at wavelength λ_i is a function of film thicknesses u_j.

$$R_{\lambda_i} = R_{\lambda_i}(u_1, u_2, u_3, \ldots\ldots\ldots\ldots u_j, \ldots\ldots u_m)$$

where i = 1,2, 3, ... n wavelength points and j = 1,2,3,...m films.

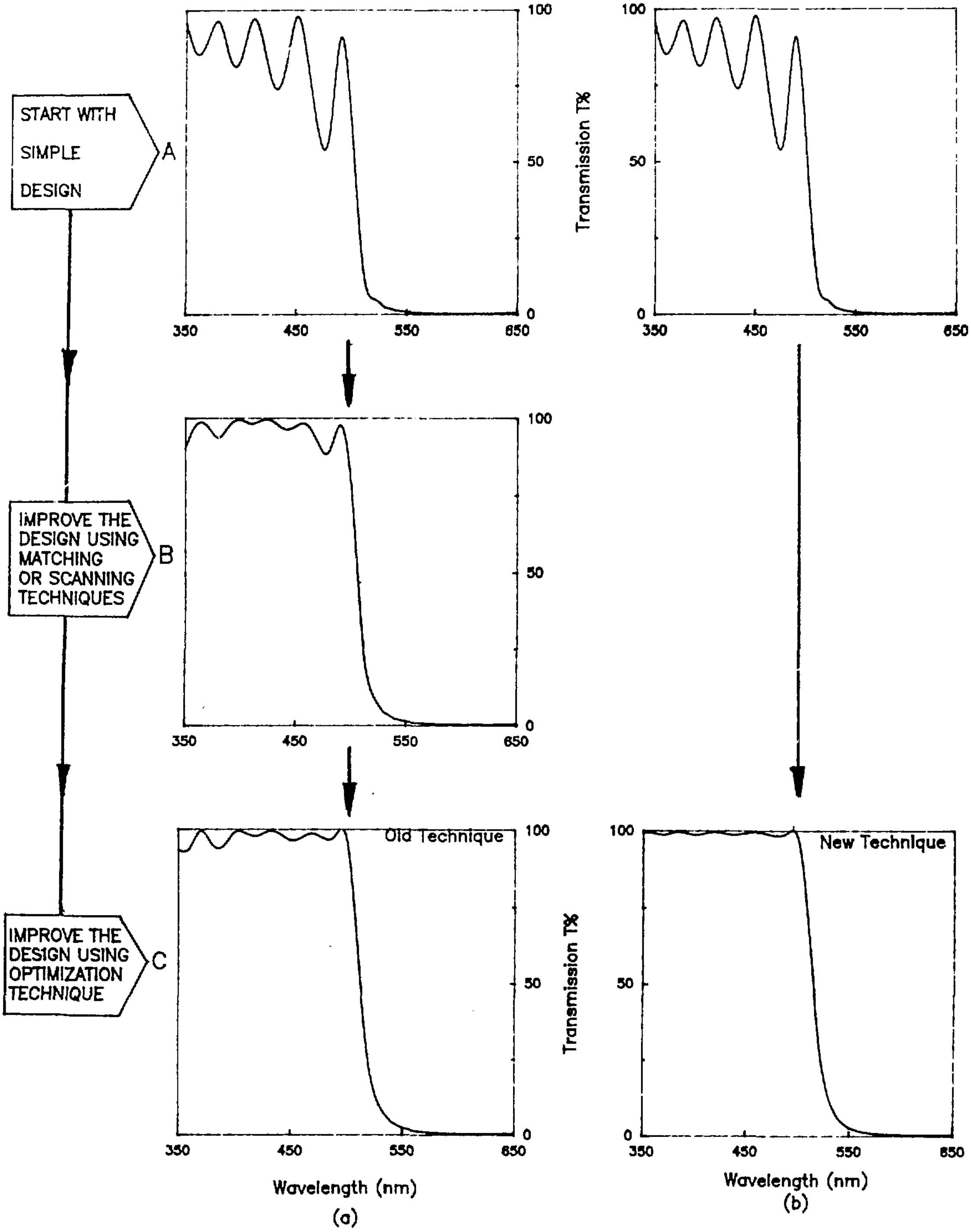

Fig.1. Working principle of thin film design procedures using the (a) Old and (b) New optimization technique to design a 15 layer edge filter .

The partial reflection derivatives $a_{ij} = \delta R_{\lambda i}/\delta u_j$ used for the old method are computed directly[23] from the reflection equation whereas for the new method they are computed indirectly[14] by giving small known film thickness increment Δv to each layer and finding out the consequent difference in reflectance ΔR which gives the corresponding derivatives as $a_{ij} = \Delta R_{\lambda i}/\Delta v_i$. Using these derivatives the optimization methods minimize the defect function ψ of the initial design in an iterative way by solving the following set of damped least squares equations[13,14].

$$\tilde{A}Ax + p^2Qx = \tilde{A}f$$

to get the required design refinement. In the above equation A is the $n \times m$ matrix, the general term of which is a_{ij}, $\tilde{A}$ is its transpose, x and f are the column vectors of the elements Δu_j and $\Delta R_{\lambda i}$ respectively and Q is a diagonal matrix with diagonal elements $q_j^2 = \Sigma a_{ij}^2$ and p is a positive damping factor.

After designing successfully number of thin film devices of varying complexities using the above old and new methods it was found that these methods have certain merits and demerits compared to one another in getting the final design to the required specifications. The difference in the design efficiencies of these two methods and the influence of the design parameter factors responsible for such differences are compared in the present studies.

6. DESIGN REFINEMENT COMPARISON OF THE OLD AND NEW DESIGN METHODS

For comparing the design refinement of multilayer optical thin film devices using the old and new methods, ten different types of multilayer thin film devices of varying specifications are designed using both the methods starting with the same initial design. For all the design examples considered here the starting

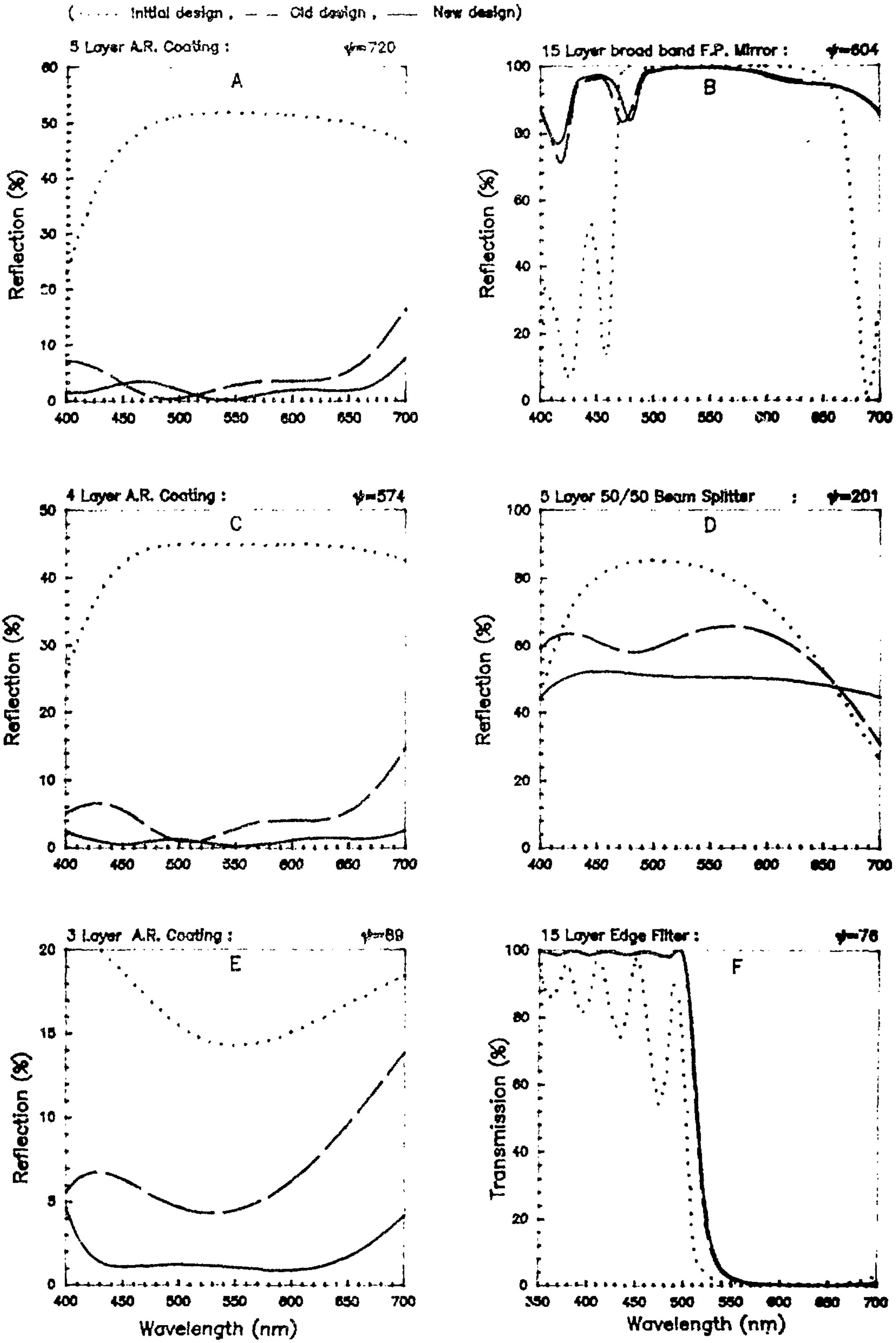

Fig. 2. Design characteristics of various designs with different initial ψ

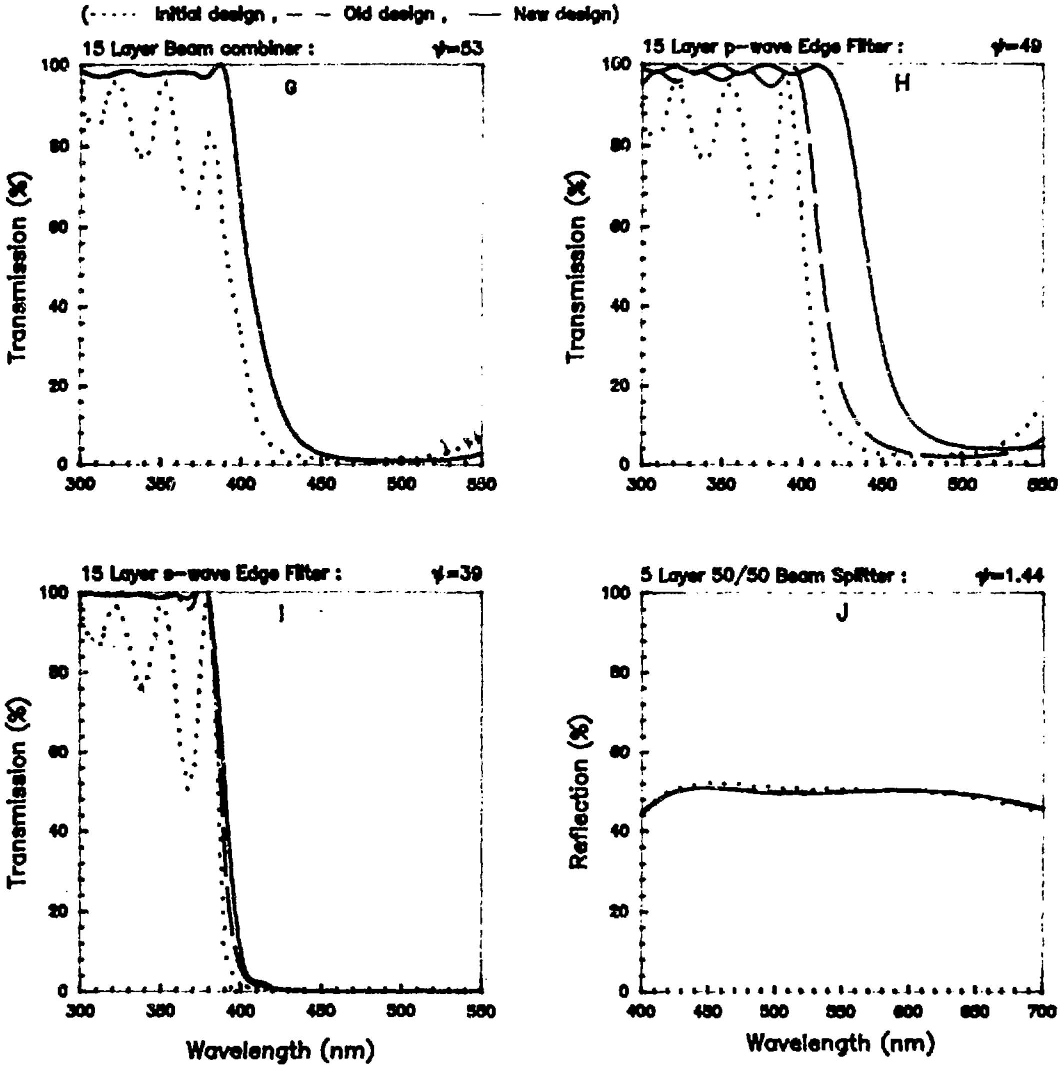

Fig. 3. Design characteristics of various designs with different initial ψ

Table 1. Optical description of different New Designs of multilayer thinfilm devices shown in Fig.2

Design	No.of	Ref.	Optical film thickness of the		
Particulars	Layer	Index	Initial Design (nm)	Old Design (nm)	New Design (nm)
Design : A					
5 Layer	Medium	1.00	Massive	Massive	Massive
A.R.Coating	1	1.38	137.5	106.0	111.4
$\theta = 0^o$	2	2.30	137.5	246.5	242.3
$\psi = 720$	3	1.38	137.5	210.0	230.1
	4	2.30	137.5	228.8	246.1
	5	1.38	137.5	258.5	209.8
	Substrate	1.52	Massive	Massive	Massive
Design : B					
15 Layer	Medium	1.00	Massive	Massive	Massive
Broad Band	1	2.30	137.5	140.5	143.2
F.P.Mirror	2	1.38	137.5	143.8	146.8
$\theta = 0^o$	3	2.30	137.5	149.8	152.2
$\psi = 604$	4	1.38	137.5	151.0	154.3
	5	2.30	137.5	150.0	153.7
	6	1.38	137.5	149.3	150.3
	7	2.30	137.5	146.5	143.3
	8	1.38	137.5	139.3	133.1
	9	2.30	137.5	130.3	125.2
	10	1.38	137.5	122.0	119.8
	11	2.30	137.5	116.0	114.9
	12	1.38	137.5	110.3	110.9
	13	2.30	137.5	106.3	108.4
	14	1.38	137.5	104.3	104.7
	15	2.30	137.5	102.3	99.1
	Substrate	1.52	Massive	Massive	Massive
Design : C					
4 Layer	Medium	1.00	Massive	Massive	Massive
A.R.Coating	1	1.38	137.5	106.3	88.4
$\theta = 0^o$	2	2.30	137.5	251.0	108.9
$\psi = 574$	3	1.38	137.5	209.3	181.4
	4	2.30	137.5	235.5	110.0
	Substrate	1.52	Massive	Massive	Massive

Table 2. Optical description of different New Designs of multilayer thinfilm devices shown in Fig.2

Design	No.of	Ref.	Optical film thickness of the		
Particulars	Layer	Index	Initial Design (nm)	Old Design (nm)	New Design (nm)
Design : D					
5 Layer 50/50	Medium	1.00	Massive	Massive	Massive
Beam Splitter	1	2.30	137.5	170.8	166.6
$\theta = 45^o$	2	1.38	137.5	125.5	124.8
$\psi = 201$	3	2.30	137.5	127.5	142.9
	4	1.38	137.5	79.3	49.6
	5	2.30	137.5	286.0	52.7
	Substrate	1.52	Massive	Massive	Massive
Design : E					
3 Layer	Medium	1.00	Massive	Massive	Massive
A.R.Coating	1	1.38	137.5	123.0	126.4
$\theta = 0^o$	2	2.30	137.5	194.0	255.8
$\psi = 89$	3	1.38	137.5	267.3	255.1
	Substrate	1.52	Massive	Massive	Massive
Design : F					
15 Layer	Medium	1.00	Massive	Massive	Massive
Edge Filter	1	1.38	150.0	88.8	90.2
$\theta = 0^o$	2	2.30	150.0	167.5	171.9
$\psi = 76$	3	1.38	150.0	161.3	162.9
	4	2.30	150.0	155.8	156.3
	5	1.38	150.0	153.0	153.6
	6	2.30	150.0	151.3	151.6
	7	1.38	150.0	150.8	151.1
	8	2.30	150.0	150.3	150.6
	9	1.38	150.0	150.5	150.8
	10	2.30	150.0	150.8	150.9
	11	1.38	150.0	151.8	152.2
	12	2.30	150.0	153.5	153.8
	13	1.38	150.0	159.3	159.6
	14	2.30	150.0	169.5	170.7
	15	1.38	150.0	173.3	170.6
	Substrate	1.52	Massive	Massive	Massive

Table 3. Optical description of different New Designs of multilayer thinfilm devices shown in Fig.3

Design	No.of	Ref.	Optical film thickness of the		
Particulars	Layer	Index	Initial Design (nm)	Old Design (nm)	New Design (nm)
Design : G					
15 Layer	Medium	1.00	Massive	Massive	Massive
UV - Visible	1	1.38	130.0	80.0	78.0
Beam Combiner	2	2.30	130.0	144.5	143.4
$\theta = 45^{o}$	3	1.38	130.0	141.8	142.2
$\psi = 53$	4	2.30	130.0	137.3	136.8
	5	1.38	130.0	134.0	134.1
	6	2.30	130.0	133.0	132.9
	7	1.38	130.0	131.8	131.8
	8	2.30	130.0	131.0	131.0
	9	1.38	130.0	131.0	131.0
	10	2.30	130.0	131.8	131.6
	11	1.38	130.0	132.3	132.5
	12	2.30	130.0	134.3	134.0
	13	1.38	130.0	138.3	138.7
	14	2.30	130.0	150.3	149.7
	15	1.38	130.0	147.8	149.8
	Substrate	1.48	Massive	Massive	Massive
Design : H					
15 Layer	Medium	1.00	Massive	Massive	Massive
P - wave	1	1.38	130.0	100.5	112.1
Edge Filter	2	2.30	130.0	148.5	210.7
$\theta = 45^{o}$	3	1.38	130.0	145.5	180.0
$\psi = 49$	4	2.30	130.0	136.5	143.9
	5	1.38	130.0	133.3	145.2
	6	2.30	130.0	132.3	138.0
	7	1.38	130.0	131.0	138.8
	8	2.30	130.0	130.5	137.5
	9	1.38	130.0	130.5	137.6
	10	2.30	130.0	131.0	140.6
	11	1.38	130.0	131.3	145.5
	12	2.30	130.0	133.0	145.2
	13	1.38	130.0	136.8	167.0
	14	2.30	130.0	146.8	178.6
	15	1.38	130.0	64.3	130.0
	Substrate	1.48	Massive	Massive	Massive

Table 4. Optical description of different New Designs of multilayer thinfilm devices shown in Fig.3

Design Particulars	No.of Layer	Ref. Index	Optical film thickness of the Initial Design (nm)	Old Design (nm)	New Design (nm)
Design : I					
15 Layer	Medium	1.00	Massive	Massive	Massive
S - wave	1	1.38	130.0	67.8	64.0
Edge Filter	2	2.30	130.0	143.5	144.2
$\theta = 45^{o}$	3	1.38	130.0	135.8	137.4
$\psi = 39$	4	2.30	130.0	132.5	133.3
	5	1.38	130.0	130.3	131.1
	6	2.30	130.0	129.3	129.5
	7	1.38	130.0	129.0	129.0
	8	2.30	130.0	128.8	129.1
	9	1.38	130.0	129.0	129.1
	10	2.30	130.0	129.0	129.6
	11	1.38	130.0	129.8	130.8
	12	2.30	130.0	131.3	132.8
	13	1.38	130.0	133.8	137.7
	14	2.30	130.0	140.3	144.0
	15	1.38	130.0	160.3	170.1
	Substrate	1.48	Massive	Massive	Massive
Design : J					
5 Layer 50/50	Medium	1.00	Massive	Massive	Massive
Beam Splitter	1	2.30	166.6	166.3	164.7
$\theta = 45^{o}$	2	1.38	124.8	125.8	127.4
$\psi = 1.44$	3	2.30	142.9	140.5	140.9
	4	1.38	49.6	46.8	44.6
	5	2.30	52.7	54.5	56.9
	Substrate	1.52	Massive	Massive	Massive

design is a simple quarter wave stack except for the design J and only two non-absorbing film materials are used for the design. The initial defect function ψ of the starting design for these design examples vary from 1.44 to 720.00 in some arbitrary units and the angle of incidence θ is taken as either 0^{o} or 45^{o}. The design characteristics obtained with both the methods for all the ten examples are shown in Fig.2 and Fig.3 and the corresponding design data are included in Tables 1 and 4. The computed performances of the initial design, the final old method design and the final new method design are shown in each plot of these figures. As can be seen in these figures the new design method gives, in general, superior and efficient designs compared to the old design method for all the examples considered here. In particular the efficiency of the new method is high for the case with relatively high initial ψ and it decreases as the initial ψ decreases. For $\psi < 76.00$ there is not much difference in the design refinement indicating that with relatively low initial ψ values both the methods are equally efficient in getting the final design and with relatively high initial ψ values the new method gives better designs compared to the old method.

7. DESIGN PARAMETERS COMPARISON OF THE OLD AND NEW DESIGN METHODS

The parameters which influence the design refinement of a multilayer thin film device in a damped least squares optimization methods are the damping factor ρ, the film thickness increment Δv, defect function ψ, wieghtage factor W and the film thickness sensitivity factor $\delta R/\delta u$. The influence of all these parameters on the design efficiency are compared for all the ten design examples using the old and new methods and the results are shown in figures 4 to 13. The efficiency of the design methods is compared in Plot A of these figures, for all the examples, where in the defect function ψ is plotted against the number of iterations N. The influence of the film thickness increment Δv on the efficiency of the method is illustrated in Plots B. The dependence of the damping factor ρ on

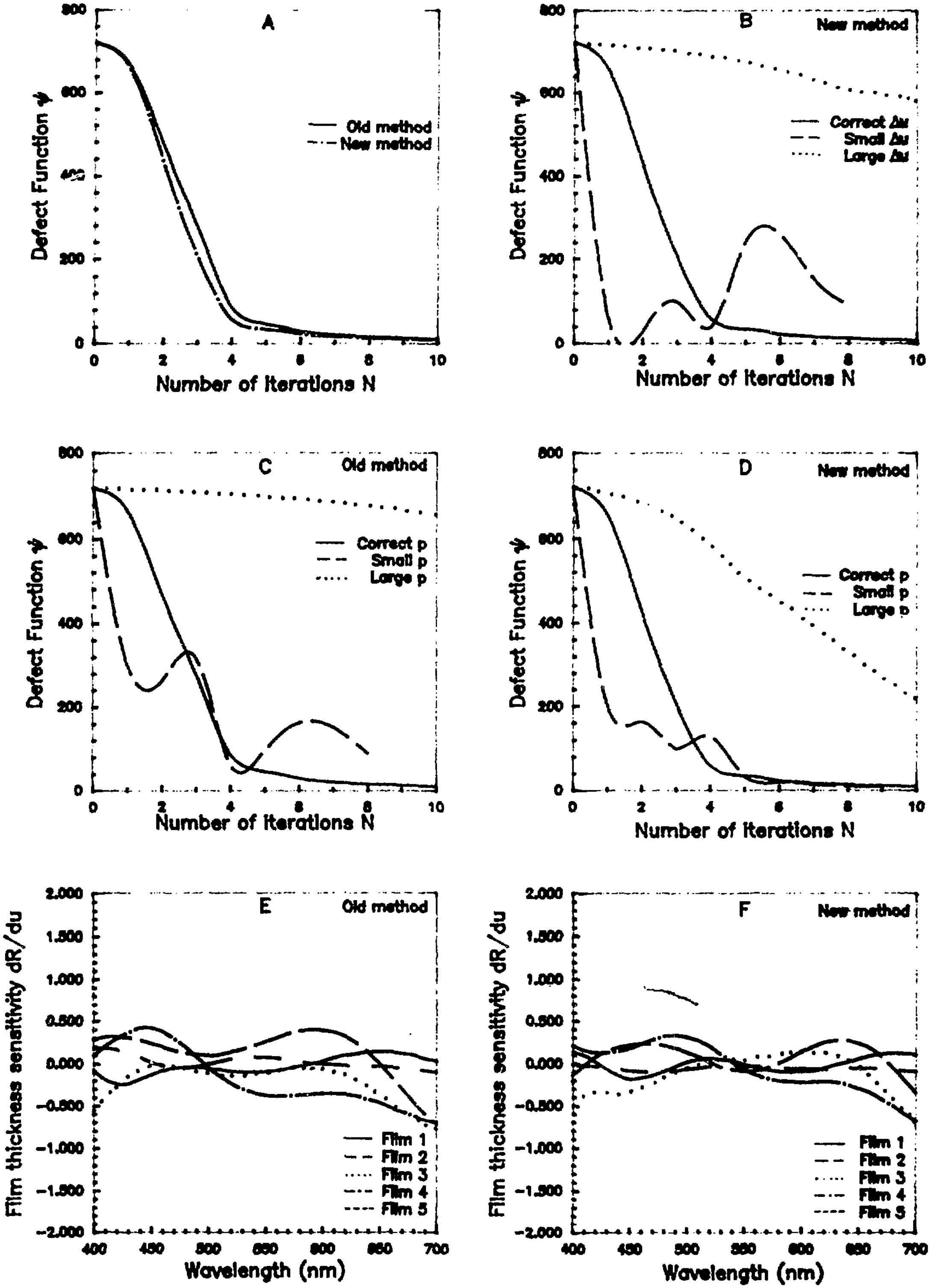

Fig. 4. Design parameter characteristics of a 5 Layer A.R.Coating
($\theta = 0$, $\psi = 720$)

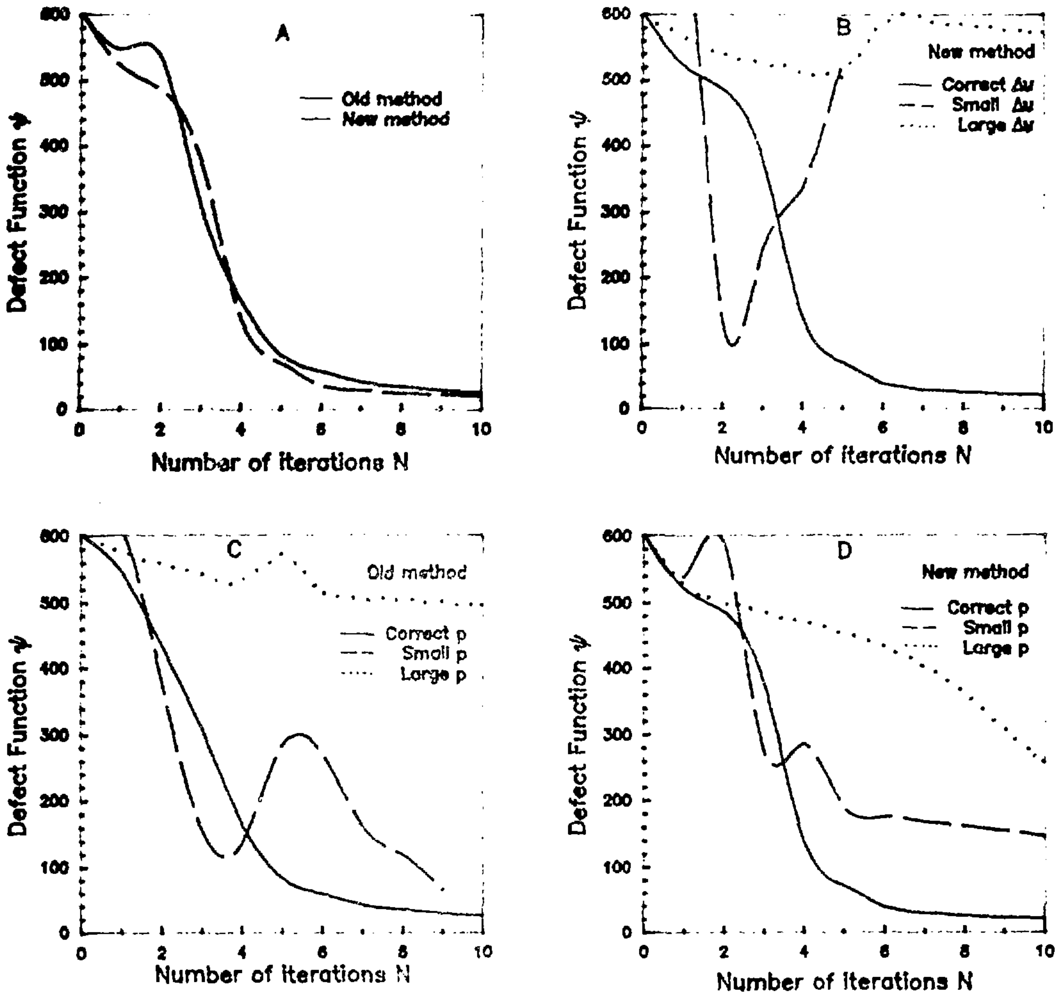

Fig.5. Design parameter characteristics of a 15 Layer Broad Band F.P.Mirror ($\theta = 0$, $\psi = 604$)

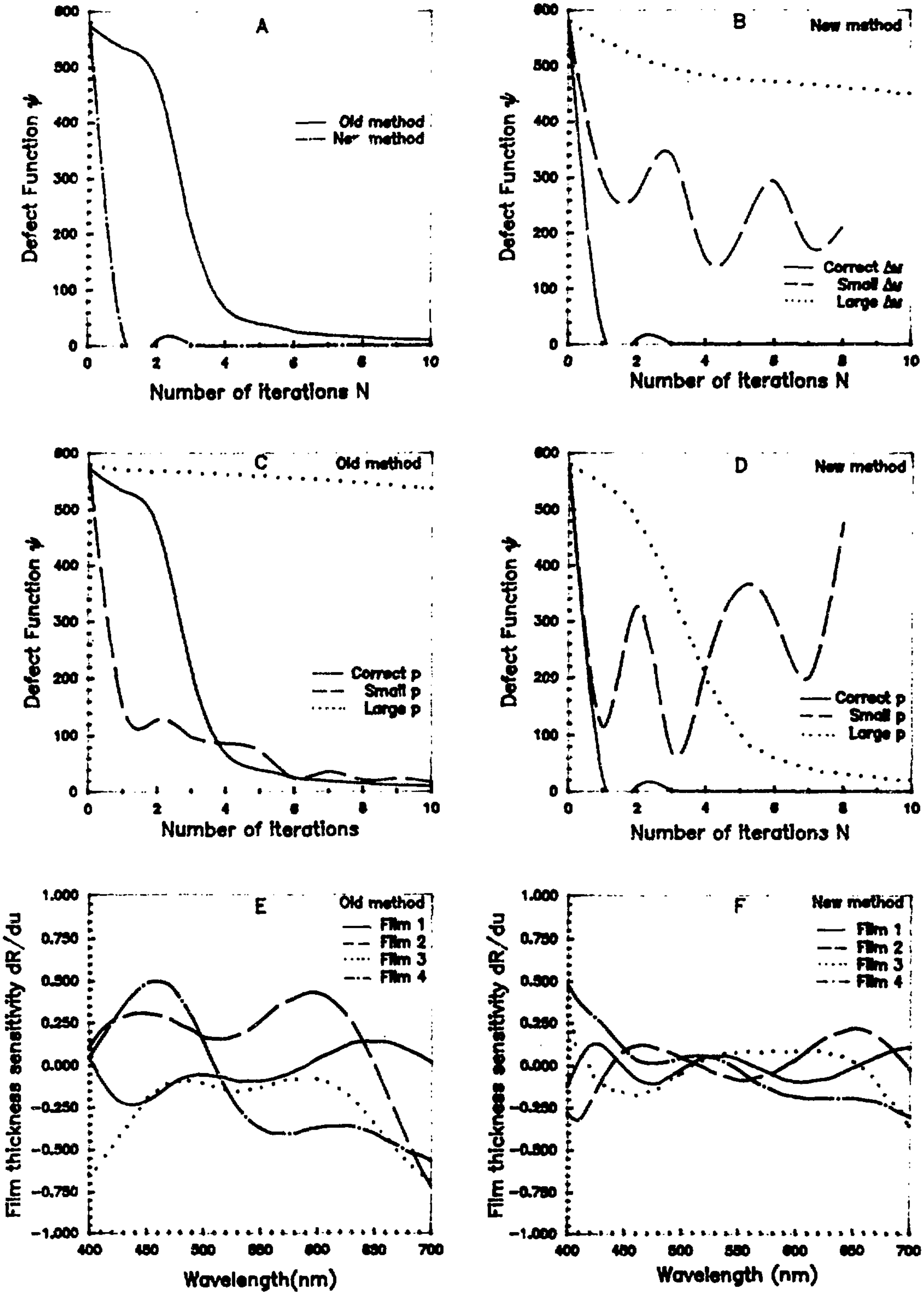

Fig.6. Design parameter characteristics of a 4 Layer A.R.Coating
($\theta = 0$, $\psi = 576$)

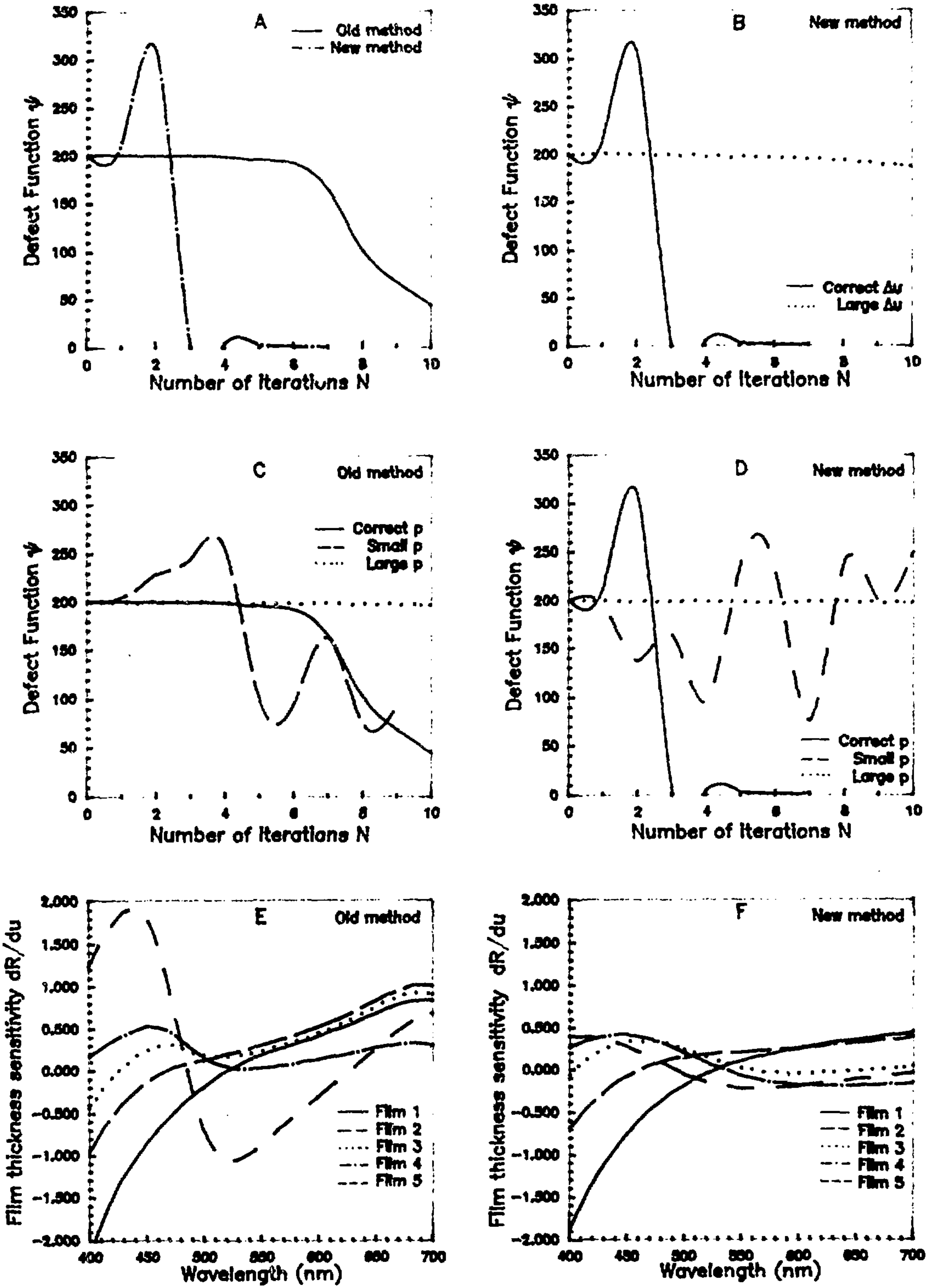

Fig. 7. Design parameter characteristics of a 5 Layer 50/50 Beam Splitter
($\theta = 45$, $\psi = 201$)

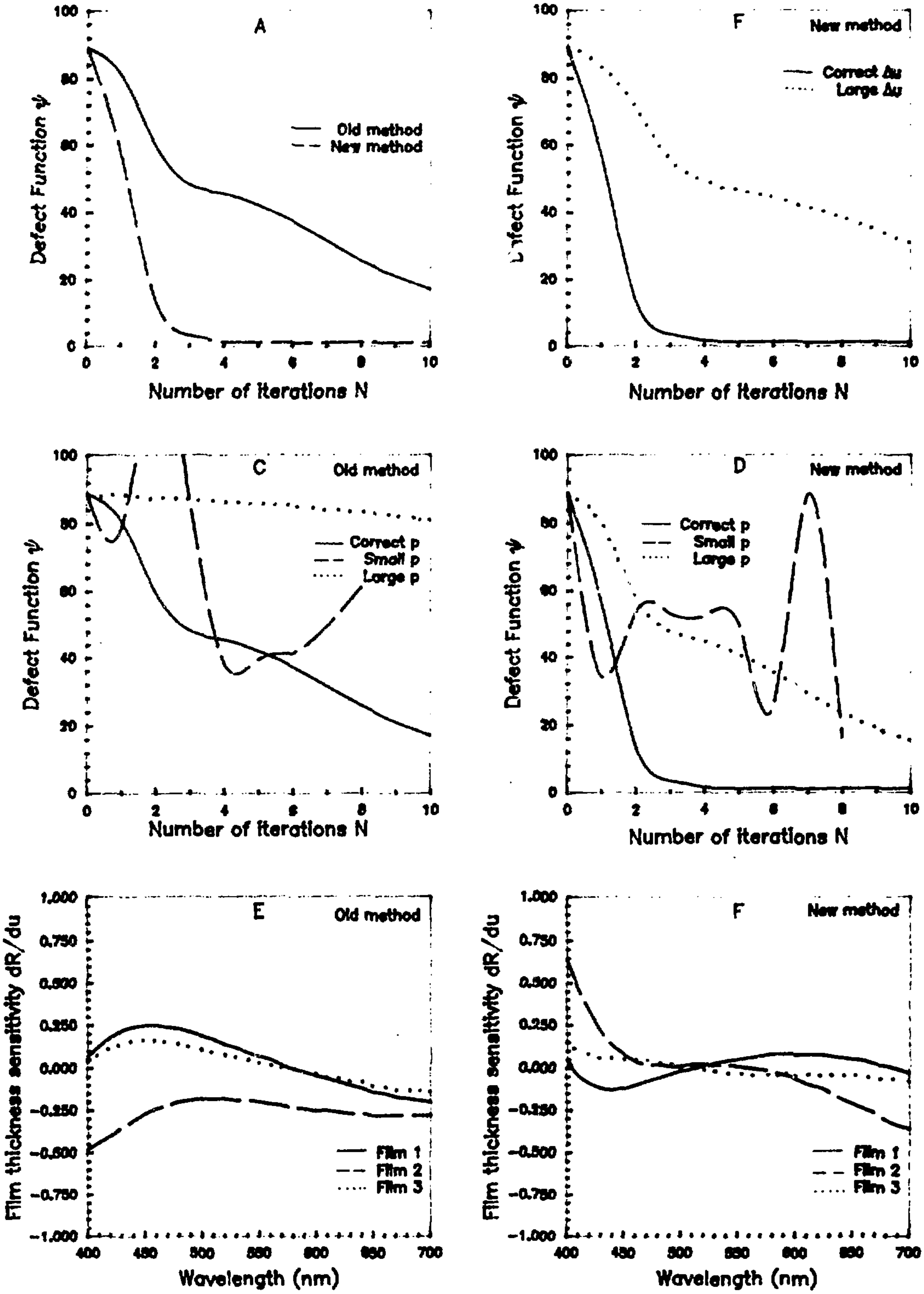

Fig. 8. Design parameter characteristics oa a 3 Layer A.R.Coating
($\theta = 0$, $\psi = 89$)

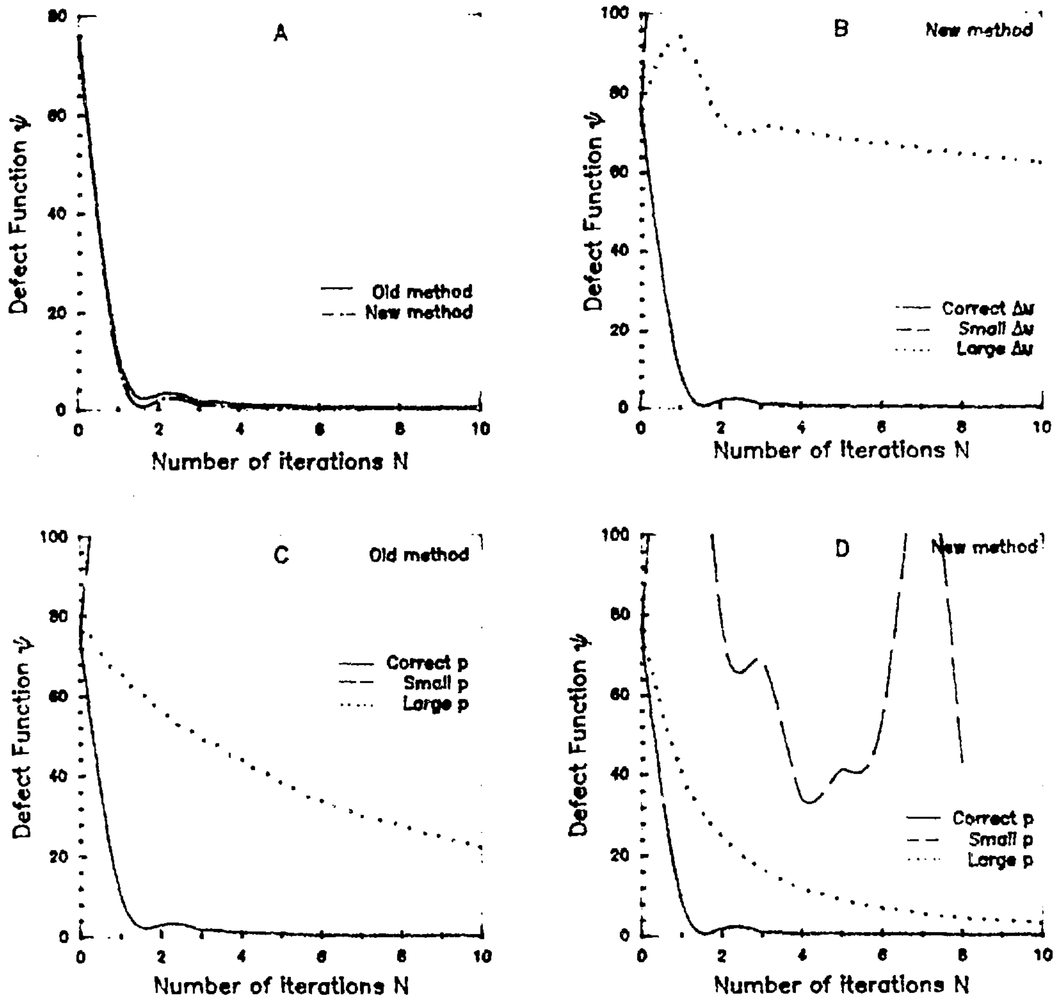

Fig. 9. Design parameter characteristics of a 15 Layer Edge Filter
($\theta = 0$, $\psi = 76$)

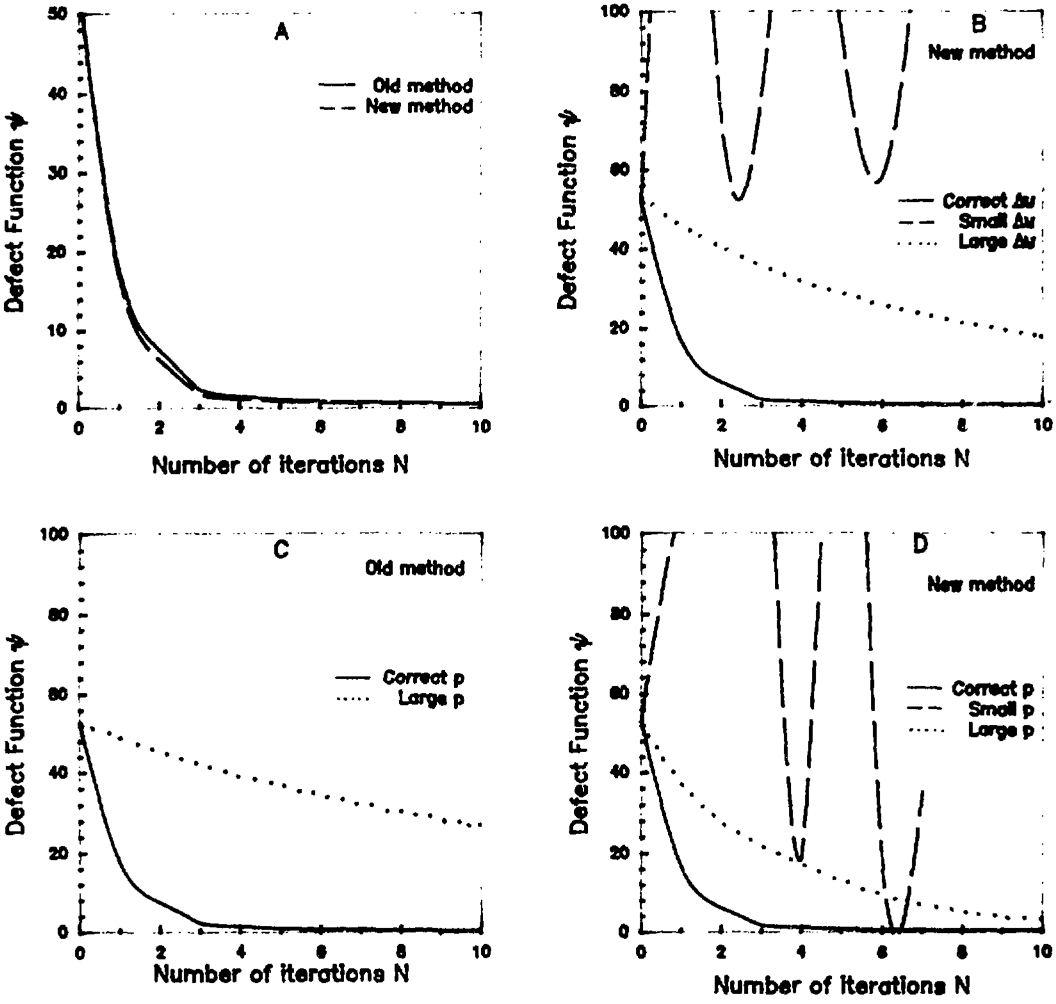

Fig.10. Design parameter characteristics of a 15 Layer Beam Combiner. ($\theta = 45$, $\psi = 53$)

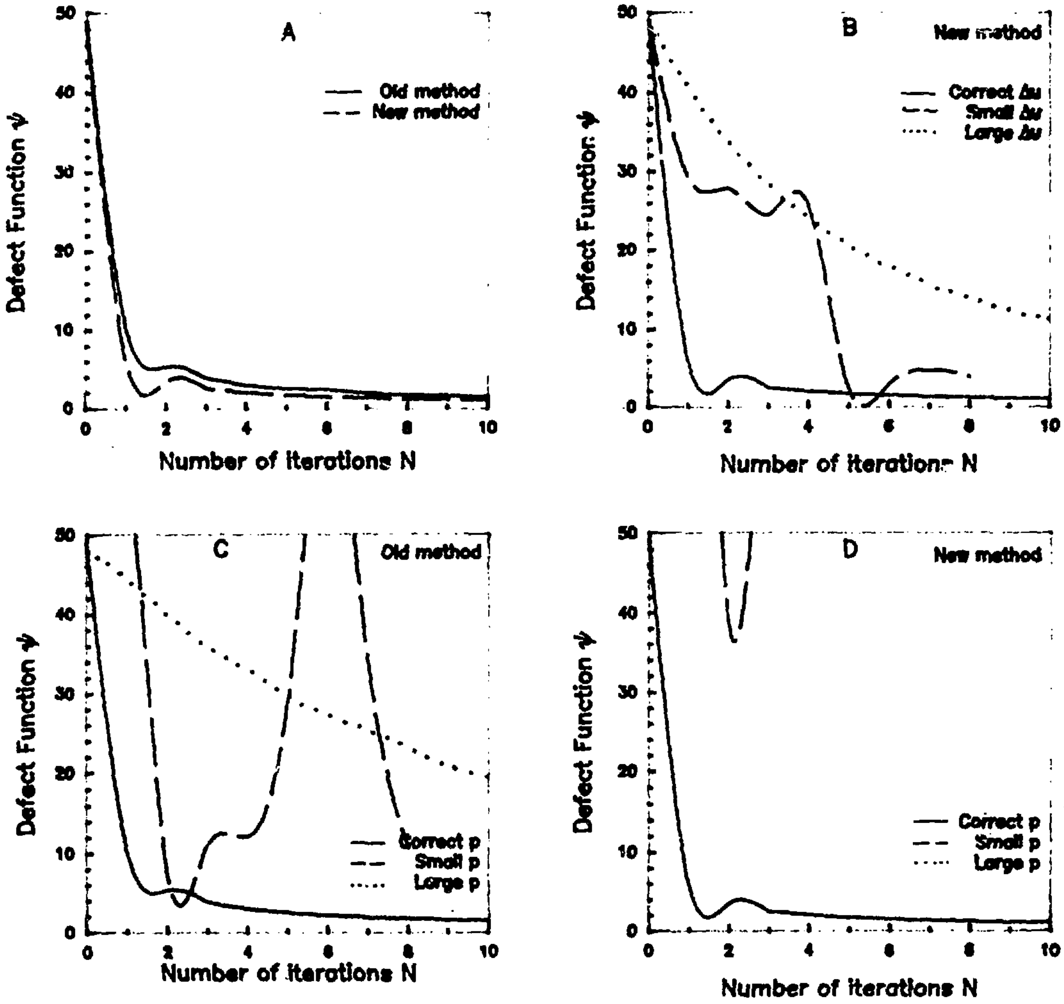

Fig. 11. Design parameter characteristics of a 15 Layer p–wave Edge Filter. ($\theta = 45$, $\psi = 49$)

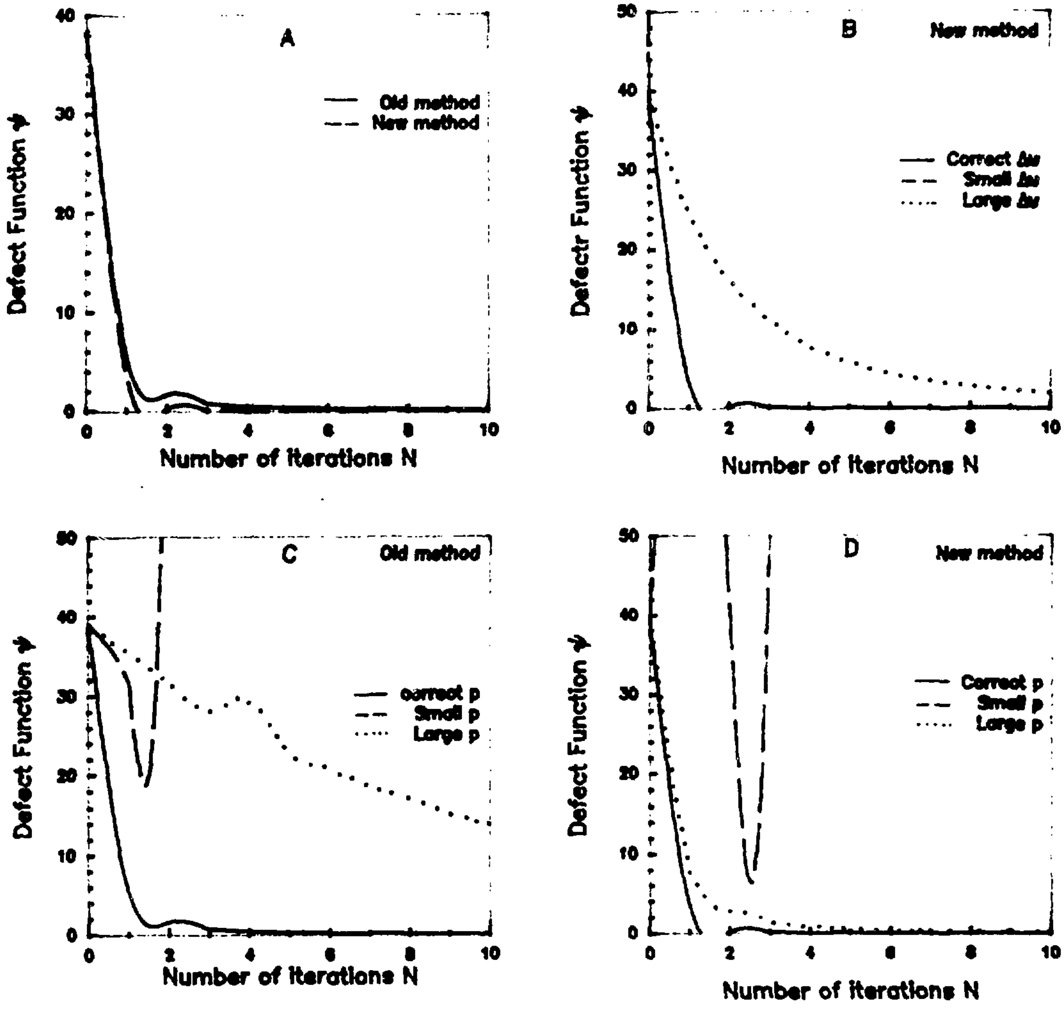

Fig. 12. Design parameter characteristics of a 15 Layer s–wave Edge Filter. ($\theta = 45$, $\psi = 39$)

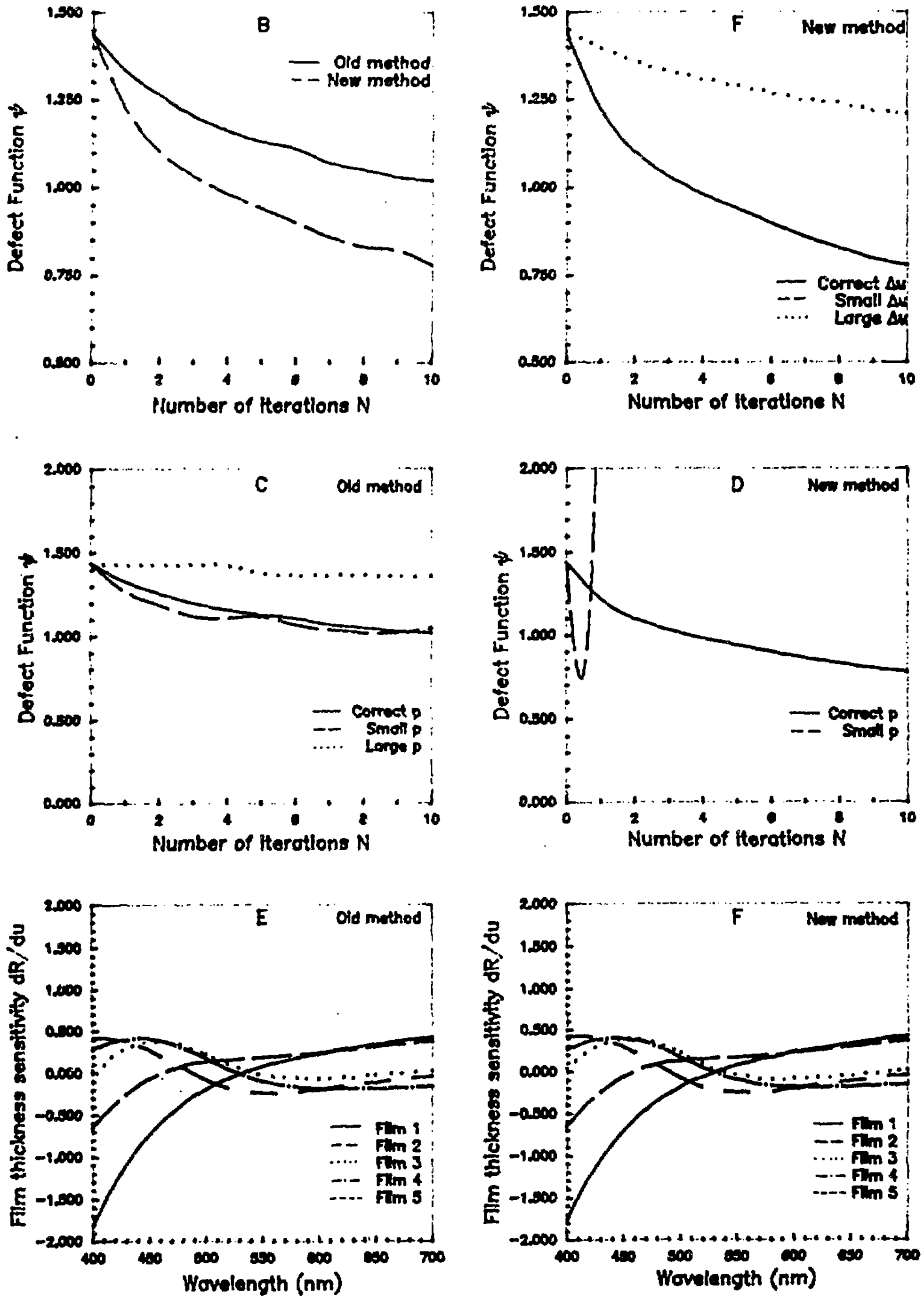

Fig.13. Design parameter characteristics of a 5 Layer 50/50 Bedm Splitter
($\theta = 45$, $\psi = 1.44$)

the degree of refinement of the old and new methods are shown in Plots C and *D* respectively. Some graphs in these figures are not seen as the corresponding points go beyond the plotting range. Finally the spectral film thickness sensitivity of the old and new methods are compared in Plots *E* and *F* respectively. For the sake of clarity these plots are shown only for the cases with number of films equal to or less than five.

The effect of the damping factor p used in the optimization methods is to have a control on the parameters Δu_j and by choosing a proper positive damping factor p, the step length $S = (\Sigma \Delta u_j^2)^{1/2}$ in parameter space can be made to lie within the approximate range of validity of a linear equation. The value of S can be increased or decreased by decreasing or increasing p. When p is zero or very small, ψ attains certain minimum and then oscillates without converging to an absolute minimum and for very large values of p , ψ converges to minimum slowly whereas for the correct p , ψ converges to real minimum in fewer iterations and remains constant indicating that further improvement of the system is not possible. Such variation of ψ with the number of iterations N is observed for both the old and new methods for all the design examples as can be seen in Plots C and *D* in figures 4 to 13. Similar behavior is observed in the variation of ψ with N for different values of film thickness increments Δv. As can be seen in Plots *B* of these figures the defect function ψ reduces to real minimum in few iterations for the correct Δv value. Whereas for small Δv the defect function reaches certain minimum and starts oscillating and for higher Δv values ψ converges to minimum very slowly.

Thus the extent of refinement of a thin film device obtained using an optimization method depends mainly on the initial defect function ψ of the starting design, the choice of damping factor p, film thickness increment Δv and weightage factors W_i. These parameters vary from one method to another and also from

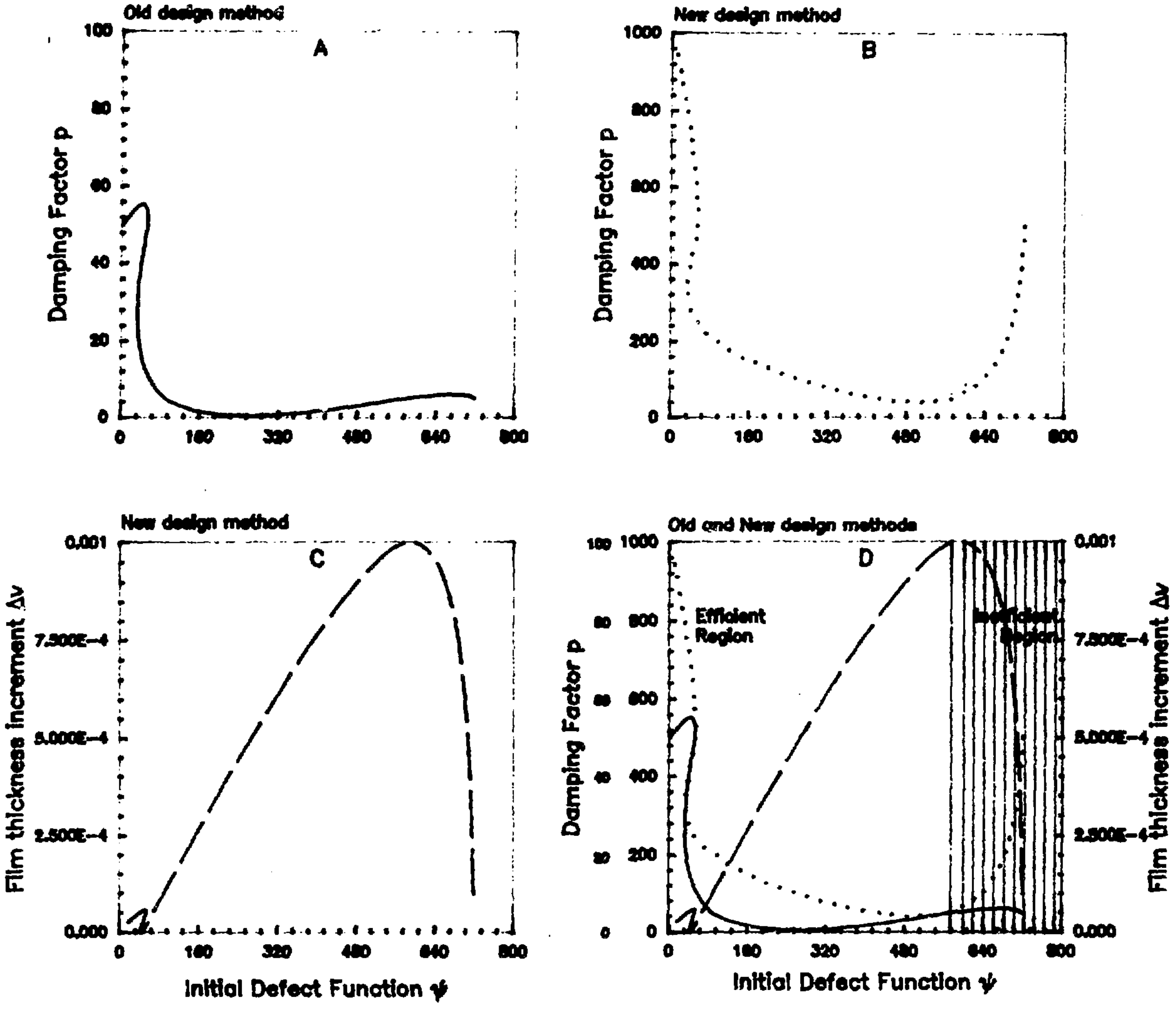

Fig. 14. Design parameter characteristics of old and new design methods

design to design. In both the methods the correct value of ρ and Δv are found in trail runs using the criteria as outlined earlier and illustrated in Plots ***C*** and ***D***. It is found from experience that the choice of ρ and Δv which depend on $\Delta R_{\lambda i}$ and W_i is not that critical and any value which is about + 50 % in error of the correct value gives reasonably good improvement in the design. But the range of correct damping factor needed for a given design is an order more for the new method compared to that of the old method as shown in Plots ***A*** and ***B*** of Fig.14 where in the variation of the correct damping factor with the initial ψ for the old and new methods respectively are shown. As can be seen in these Plots the damping factors needed for both the methods decrease initially as ψ increases and at high ψ values the required damping factor increases. Whereas in the case of film thickness increment parameter Δv , the correct Δv needed increases initially as ψ increases and at high ψ values the required Δv decreases as shown in Plot ***C*** of Fig.14. The plots of both the damping factors and film thickness increment needed versus initial defect function are shown in Fig.14D, which shows clearly the efficient region of ψ where the method works efficiently with proper choice of the parameters. The plot also shows the inefficient region of ψ where both the methods fail to give the required design efficiently with any parameter values.

The final parameter for the present comparison is the spectral film thickness sensitivity factors $\delta R/\delta u$ which are very useful during the fabrication stage of the device. The film thickness sitivity of all the films of the final designs obtained with the old and new methods are compared in Plots ***E*** and ***F*** of figures 4 to 13 which show that film thickness sensitivity of the devices designed with the new method are less compared to those of the old method.
method.

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