

Fitting refractive-index data with the Sellmeier dispersion formula

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The fitting of measured optical index data to the Sellmeier dispersion formula, using the variable projection algorithm, is described. Examples of fits obtained by this method to several Schott optical glasses and non-glass materials are given.

I. Introduction

This paper describes a method for the fitting of optical index data to the Sellmeier dispersion formula. The work described began in 1964. It was shown in the 1960s that the Sellmeier formula was suitable for accurately fitting both glass and nonglass¹⁻³ materials. This paper describes a program, INFIT, which uses a new curve-fitting procedure and which is applicable to both types of material.

In Sec. II we discuss the need for curve-fitting index data. In Sec. III we present the Sellmeier formula and discuss the specific problems involved in fitting it. In Sec. IV we describe the new algorithm used in the recent continuation of the work of Ref. 3. In Sec. V we describe some specific features of the INFIT program and present our numerical results, comparing them with results taken from the literature when possible. Finally, as a postscript, Sec. VI gives a comparison of INFIT with the results of four additional references discovered after the main body of this paper was written.

II. The Problem

References 1 and 2 cover most of the reasons curve-fitting index data are useful to do and the physical justification for using the Sellmeier formula for this purpose. In addition, Herzberger has pointed out the relationship between fitting dispersion data and the correction of chromatic aberrations in lens systems.⁴ It might also be of interest to relate the reasons for our interest in this subject. At the time of preparing Ref.

3, Itek was primarily in the business of manufacturing large aperture high-quality refractive lenses for use in visible light. As is well known, chromatic aberration is an important problem associated with such lenses. Since all refractive materials exhibit dispersion, the only way to correct the chromatic aberration is with a weighted combination of the dispersions of different materials, thus obtaining a composite material of more or less zero dispersion. The accuracy with which this has to be done is equal to a fraction of the difference in physical path times the optical index for any two rays contributing to a given image point. Since the measure for this difference is the wavelength of light, the various dispersion curves have to be known very accurately, in particular, about 1 in the sixth place for the most critical applications in visible light.⁵

Aside from the problem of making glass to such a high standard, measuring its optical properties this accurately is itself an extremely difficult problem. Indices are measured in carefully controlled conditions using certain discrete wavelengths corresponding to stable, strong, isolated, etc. absorption or emission lines. The Schott Optical Glass Co., who was our major supplier of glass because of the reliability not only of their glass quality but also of the data they furnished for it, gave dispersion data in their catalog to five-place accuracy at 10-12 wavelengths from 1.0 to 0.36 μm . At that time, they did not provide data for a dispersion formula. The catalog data were an average of measurements over a more or less number of lots of the glass, depending on its relative popularity. For a specific purchase, they provided a melt sheet consisting of measurements on that specific batch to six-place accuracy over a lesser number of wavelengths. Thus, if the lens was to be used over a short-wavelength band, the dispersion would be specified directly only over a relatively small number of wavelengths, and an error in only one of these could be disastrous. In effect, then, such a lens, because of its extreme sensitivity to the dispersion data, could be considered as a device for checking the dispersion data,

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except that it would be an extremely expensive device for such a purpose.

Two approaches suggested themselves for ensuring against the possibility of an error in dispersion data. One was to try to measure the data independently, and a small laboratory was actually set up to do this. The other was to apply curve-fitting techniques on the data to smooth the errors and indicate their magnitude. The latter approach would have been useful even without the concern for errors, since we needed the index data at intermediate wavelengths in order to efficiently integrate the lens performance effects over wavelength. Because of the extreme sensitivity of the performance of the lens to the data and the relatively large separation of the measured points, interpolation based on a power series approach would not have sufficed. As far as the measurement option was concerned, this rapidly turned into a fiasco, since, after our laboratory rejected some glass samples and they were returned to Schott, Schott sent them back insisting they were as claimed. Thereupon, applying our newly developed fitting method to both sets of data, we determined that the Schott data were indeed correct.

III. Sellmeier Dispersion Formula

There are several dispersion formulas available that could have been used for fitting index data. These include, as the most important, those due to Hartman, Conrady, Herzberger, Schott Optical Glass, Inc., and Sellmeier. Some of these, such as the Conrady, Herzberger, and Schott formulas, are linear in the fitting constants, which means they can be fitted easily using the classical least-squares procedure. This was an important consideration prior to the availability of today's powerful electronic computers. However, from what has been said above, it is clear that fitting accuracy should be the dominant consideration in choosing a dispersion formula. From the results given here and elsewhere, the Sellmeier formula is not only the most accurate of the formulas mentioned, but it is capable of fitting index data to an accuracy fully consistent with both the present ability to measure such data and the accuracy needed for most applications.

The Sellmeier formula is given by

$$N^2 = 1 + \sum_{j=1}^k \frac{A_j \lambda^2}{\lambda^2 - B_j^2}; \quad (1)$$

N is the optical index at wavelength λ , and k , A_j , and B_j are the constants to be determined by the fitting process. The difficulty in fitting Eq. (1) is due to the indeterminacy of the number of terms k and the nonlinearity with respect to the B_j values. From Refs. 2 and 3 it has been found that $k = 3$ is generally a necessary and sufficient value for satisfactorily fitting almost all the materials in practical use in their main transparent region. However, even when k is known, there are several difficulties in solving for the B_j constants. These are choice of starting values, iteration to a solution, and degeneracy.

The choice of starting values is not too critical as such. The problem lies in that the B_j values cannot get too

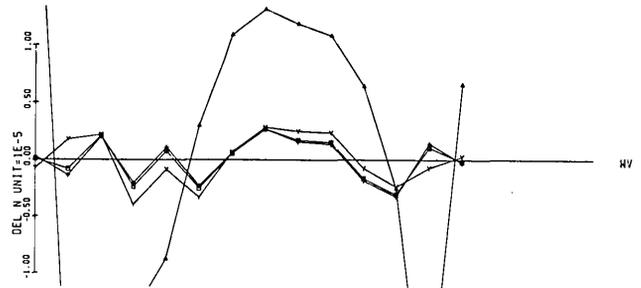


Fig. 1. Fitting error, BK7—fourteen points from 0.37 to 1.01 μm : \blacktriangle = optimum two-term fit; $+$ = three-term fit, $B_2 = 0.17$; Y = three-term fit, $B_2 = 0.26$; \square = optimum three-term fit.

close to or lie within the transmission band of the material, so that whatever one chooses for the initial configuration of absorption bands has to remain that. Here again, it has been found that for all the three-term cases tried, the optimum configuration is two absorption bands on the ultraviolet (UV) side and one on the infrared (IR) side of the transmission band (Case A of Ref. 2). In Ref. 2 a fairly elaborate procedure is given to obtain the three-term formula starting values after a two-term fit is obtained. In both Ref. 3 and this paper it has been found that almost any values can be used for starting values, provided they are not too close together and are not too close to the transmission band of the material. For glass, we always start with $B_1 = 0.1$, $B_2 = 0.22$, and $B_3 = 4$. The procedure for nonglass materials is described in Sec. V; the choice of starting values for these is also fairly arbitrary.

The basic iteration procedure used in Refs. 2 and 3 is nonlinear least squares using Newton's method. The major cause of failure in the iteration is degeneracy, where the influence of one or more of the B_j terms on the state of fit becomes small. This can occur in several conditions: (1) an insufficient number of measured data points; (2) insufficient accuracy in the measurements, where incidently the accuracy of the wavelength data has to be consistent with that of the index measurement; (3) the wavelength band defined by the data points is too narrow; and (4) an absorption band is weak. One is apt to have more trouble with the first and third conditions with glass because the transmission band for glass is naturally narrow and there tends to be a lack of suitable wavelength sources. On the other hand, the second condition is generally a problem with nonglass materials because most of the data points are in the nonvisible spectrum and because the optical quality of many nonglass materials is not that high. The fourth condition seems to be a problem most often in glass cases. If the IR band is weak, the corresponding B_j value has a tendency to go to infinity, with a corresponding large A_j value. We take care of this by putting a limit on how large the IR B_j value can get and bounding it when it tries to exceed that. We also have found that for crown (low dispersion) glasses, the UV band closest to the transmission band of the glass tends to be weak. This is illustrated in Fig. 1. The two curves marked with a $+$ and Y represent a three-term fit to the crown glass, BK7, in which the value of B_2 is fixed at

0.17 and 0.26, respectively. As can be seen, there is little difference between these two solutions, or for that matter between these and the optimum solution, which is marked by boxes. However, the curve marked with triangles, which is the best two-term fit, shows that a three-term fit is necessary. In the program of Ref. 3, we circumvented this form of degeneracy by obtaining a sequence of three-term fits in which the B_2 values were fixed at a set of discrete values, and then fitting the resulting merit values to a quadratic to obtain the minimum with respect to B_2 .

IV. Variable Projection Algorithm^{6,7}

The procedures used in Refs. 2 and 3 are each capable of solving the fitting problem they were designed for and, with additional modifications, may also be adaptable to the more general case. However, since then a more powerful algorithm, specifically suited to the general curve-fitting problem, has become available. This gives promise of being able to solve the general index fitting problem in a unified way, this is, with a minimum of special *ad hoc* procedures, and so we have incorporated this variable projection (VP) algorithm into a new program called INFIT. The basic idea of this method follows.

The general curve-fitting problem can be stated as follows. Given the m component vectors λ and \mathbf{N} that represent the data, the l component vector α and the n component vector \mathbf{a} , which are the fitting parameters, the $m \times n$ matrix of functions, $\Phi(\alpha, \lambda)$, and the m component residual vector $\mathbf{r}(\mathbf{a}, \alpha)$, we want to fit the data to the functions in the least-squares sense or, in other words, obtain

$$\min_{\mathbf{a}, \alpha} \|\mathbf{r}(\mathbf{a}, \alpha)\|^2 = \|\mathbf{N} - \Phi(\alpha, \lambda)\mathbf{a}\|^2. \quad (2)$$

The norm $\|\dots\|$ is the Euclidean norm (the square root of the sum of squares). If α is fixed, this gives

$$\min_{\mathbf{a}} \|\mathbf{r}(\mathbf{a})\|^2 = \|\mathbf{N} - \Phi(\lambda)\mathbf{a}\|^2, \quad (3)$$

which is just a linear least-squares problem whose solution⁸ is

$$\mathbf{a} = \Phi^+\mathbf{N}, \quad (4)$$

where Φ^+ is the generalized inverse of Φ , which if Φ has the rank n , is given by $(\Phi^T\Phi)^{-1}\Phi^T$, T indicating the transpose. The more general nonlinear problem, Eq. (2), has to be solved by means of a Newton method iteration. Therefore, let us expand the perturbed residual vector by a Taylor series up to the linear terms

$$\mathbf{r}(\mathbf{a} + d\mathbf{a}, \alpha + d\alpha) = \mathbf{r}(\mathbf{a}, \alpha) - \left(\Phi, \frac{\partial\Phi}{\partial\alpha} \right) (d\mathbf{a}, d\alpha)^T. \quad (5)$$

Then Eq. (2) becomes

$$\min_{d\mathbf{a}, d\alpha} \|\mathbf{r}(\mathbf{a}, \alpha) - \left(\Phi, \frac{\partial\Phi}{\partial\alpha} \right) (d\mathbf{a}, d\alpha)^T\|^2, \quad (6)$$

which, again being linear, has the solution

$$(d\mathbf{a}, d\alpha)^T = \left(\Phi, \frac{\partial\Phi}{\partial\alpha} \right)^+ \mathbf{r}(\mathbf{a}, \alpha). \quad (7)$$

Then \mathbf{a} and α are incremented by $d\mathbf{a}$ and $d\alpha$, and this is repeated until no further improvement results.

Note that, because the two variables α and \mathbf{a} occur as a product in Eq. (2), the problem of optimizing with respect to both sets of parameters is nonlinear, that is, we have lost the advantage of the linearity in \mathbf{a} . The basic idea of the VP algorithm is to preserve the separation of the parameters into linear and nonlinear sets. Thus, if we consider \mathbf{a} in Eq. (4) as a function of α , Eq. (2) becomes

$$\min_{\alpha} \|\mathbf{N} - \Phi(\alpha)\Phi^+(\alpha)\mathbf{N}\|^2, \quad (8)$$

which is a nonlinear problem in α alone. The operator $P = \Phi\Phi^+$ is the projection operator onto the space spanned by the columns of Φ , which is how the algorithm gets its name. To solve Eq. (8) by nonlinear least squares as in Eqs. (5)–(7), we need the derivative of this projection operator with respect to α . If the symbol \mathbf{D} indicates the derivative operator and \mathbf{I} is the unit matrix, this is given by

$$\begin{aligned} \mathbf{D}P &= \mathbf{Q} + \mathbf{Q}^T, \\ \mathbf{Q} &= (\mathbf{I} - P)(\mathbf{D}\Phi)\Phi^+. \end{aligned} \quad (9)$$

The theoretical and computational details of the algorithm can be found in the indicated references.

V. Description of INFIT Program and Numerical Results

The details of the implementation of the VP algorithm in the INFIT program are as follows. For glass, a three-term formula is used exclusively with starting values as indicated above. For nonglass materials, we start with a two-term formula, and then successively add additional UV terms, the additions being made only if substantial improvement resulted from the last case. Finally, an attempt at adding a second IR term to the best previous case is made. The starting B_j values of the UV terms are (1) an approximation to the UV B_j value closest to the transmission band of the material is obtained by fitting one term of the Sellmeier formula to several data points on the UV end of the band, and (2) successive UV B_j values are set at half of the value of the previous B_j . One IR B_j value is always started at double the longest wavelength used. If a second IR term is being used, its B_j value is fixed at the upper boundary for the IR terms, 100 times the longest wavelength input. The squares of the B_j values are the actual variables used in the computations, and in addition, because the IR B_j values can become numerically large, the squares of their reciprocals are used as the variables.

The data for five Schott glasses⁹ were fitted using the INFIT program. The index values used are given in the catalog to five-decimal-place accuracy over 15–18 wavelengths from 0.36 to 2.32 μm . The VP algorithm as described above obtained the optimum three-term fit for all these cases without the use of any other special procedure, as for example, dropping one of the UV denominator coefficients, as was sometimes necessary in the old program. The data used in the old program

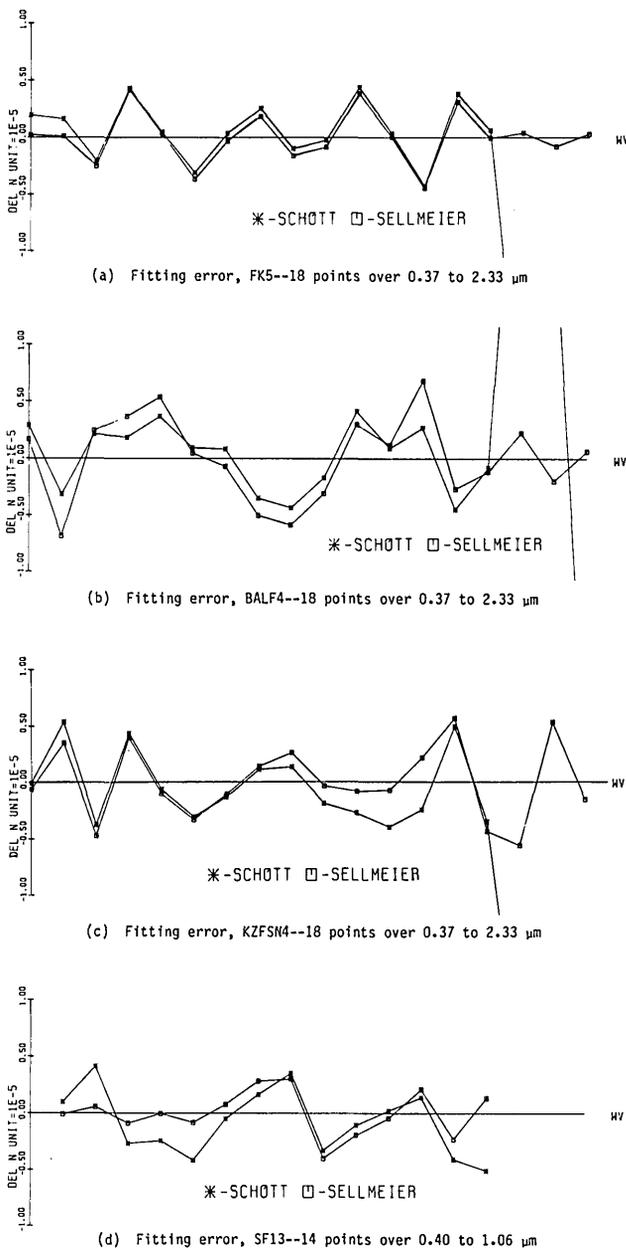


Fig. 2. Results from INFIT program for four glasses.

Table I. Sellmeier Coefficients for Selected Schott Glasses

Glass	A1	A2	A3
	B1	AB	B3
FK5	1.03630719	1.52107703e - 1	9.13166269e - 1
	7.76227030e - 2	1.38959626e - 1	9.93162512
BALF4	1.25385390	1.98113511e - 1	1.01615191
	8.56548405e - 2	1.73243878e - 1	1.08069635e + 1
KZFSN4	1.38374965	1.64626811e - 1	8.5913757e - 1
	9.48292206e - 2	2.01806158e - 1	8.28807544
SF13	1.68311631	2.28813100e - 1	5.17482874e - 2
	1.17985319e - 1	2.49318140e - 1	2.67826498

were over the wavelength range from 0.36 to 1.014 μm . The fact that the new data are available at four additional wavelengths, from 1.06 to 2.32 μm , is not the reason for the improved performance, because the case of Fig. 1, used to illustrate the problem of degeneracy, and that of Fig. 2(d), were also over this smaller range. The coefficients obtained for four of the glasses are given in Table I, and the resulting fitting errors are plotted in Figs. 2(a)-(d).

To more clearly display the errors, the data points in these plots are shown as equally spaced in wavelength, even though they are not. This is justified by the fact that the errors are independent of each other. In the same diagram we have also plotted the error in the Schott formula as given in the Schott catalog. These curves illustrate that the two formulas are equally valid over the 0.36-1.014- μm range, but the Sellmeier formula works well over the extended range from 1.014 to 2.33 μm , whereas the Schott formula exhibits large errors.

The INFIT program was also used to fit the data for eleven nonglass materials taken from various sources, as summarized in Table II. For some of these materials, it was necessary to limit the solutions for the B_j values. Since, as mentioned earlier, the actual variable used in the iteration is B_j^2 or $1/B_j^2$, these values cannot be less than zero. Also, they cannot be such that they fall in the transmission band of the material. In addition, it is desirable for the logic of the coding that the B_j terms not change their numerical order. These conditions impose positive and negative constraints on the solutions obtained for the B_j terms. In all cases, the unconstrained solution was obtained first. This was examined for constraint violations of the types described

Table II. Eleven Nonglass Materials Whose Data were Fitted to the Sellmeier Formula

Name	Symbol	No. of points	Wavelength band, μm	Accuracy ^a	Reference
Zinc sulfide	ZnS	59	0.42-18.2	3	10, 11
Zinc selenide	ZnSe	56	0.54-18.2	4	10
Fused silica	SiO ₂	60	0.21-3.71	5	12
Germanium	Ge	17	2.06-13.0	4	13
Silicon	Si	30	1.36-11.0	4	14
Fluorite	CaF ₂	46	0.23-9.72	5	15
Barium fluoride	BaF ₂	45	0.26-10.4	5	16
Sapphire	Al ₂ O ₃	46	0.26-5.58	5	17
Arsenic trisulfide	As ₂ S ₃	26	0.58-11.9	5	18
Cesium iodide	CsI	54	0.30-53.1	5	19
Thallium-bromide-iodide	KRS5	38	0.58-39.4	5	20

^a Indicates the number of decimal places to which the data were given.

Table III. Sellmeier Coefficients for Eleven Nonglass Materials

Material	A1 B1	A2 B2	A3 B3	A4 B4
ZnS	3.60981117 1.69807804e - 1	4.90409060e - 1 3.02036761e - 1	2.73290892 3.38906653e + 1	
ZnSe	4.45813734 2.00859853e - 1	4.67216334e - 1 3.91371166e - 1	2.89566290 4.71362108e + 1	
SiO ₂	6.63472443e - 1 6.65176613e - 2	4.40647918e - 1 1.15015076e - 1	8.99007061e - 1 9.90316809	
Ge	1.47587446e + 1 4.34303403e - 1	2.35256294e - 1 1.26245893	-2.48822748e + 1 1.30200000e + 3	
Si	1.06684293e + 1 3.01516485e - 1	3.04347484e - 3 1.13475115	1.54133408 1.10400000e + 3	
CaF ₂	3.37600771e - 1 0.00000000	7.01104586e - 1 9.36732830e - 2	3.84781530 3.46438880e + 1	
BaF ₂	1.00630737 7.55931756e - 2	1.43785573e - 1 1.32364522e - 1	3.78847824 4.61709395e + 1	
Al ₂ O ₃	5.31480751e - 1 2.17947151e - 2	1.55060106 1.03348342e - 1	5.28958116 1.79393145e + 1	
As ₂ S ₃	4.07205767 2.08841706e - 1	7.44196974e - 1 3.95964740e - 1	9.88377784e - 1 2.77481958e + 1	
CsI	1.29377099 1.19603583e - 1 1.19456223 1.12551827e - 1	7.43072510e - 1 2.03559339e - 1 8.42745359e - 1 2.00665347e - 1	2.91889631 1.51026230e + 2 1.30468586e - 1 8.03225264e + 1	3.12612881e + 3 5.31200000e + 3
KRS5	3.75415165 2.08331008e - 1	9.09002797e - 1 3.77160136e - 1	1.25434711e + 1 1.65646424e + 2	

above, which, if present, were dealt with by suitably bounding the solution.

For all eleven materials in the two-term fit cases, only silicon required any limiting action, and this was a positive bound violation. The IR numerator term, A₂, for both Si and Ge, ended up negative, which while unphysical, was accepted because it still yielded a smooth interpolation. This effect probably occurred because both materials have very low dispersions in the long-wavelength end of their spectra, and their data are difficult to measure.

In the three-term fit cases, seven of the materials did not require any limiting action. The Si and Ge materials had positive bound violations; CaF₂ and CsI had negative bound violations for their B₁ coefficients that wanted to become negative. Coefficient B₁ for CaF₂ ended up at zero. Coefficient A₃ for Ge ended up negative as in the two-term case. All the cases for four-term fits involving three UV terms and one IR term required both types of limiting action. Two of these cases failed, and the remainder converged to solutions with no improvement over the three-term fits. The four-term fits involving two UV terms and two IR terms all succeeded, but only one case, CsI resulted in any improvement, and this was marginal.

Therefore, based on the above results, it again seems to be generally true that a three-term Sellmeier formula is adequate for all cases. Table III gives the coefficients for the optimum fits obtained in the above, and Figs. 3-14 show the resulting errors. (A comparison of the

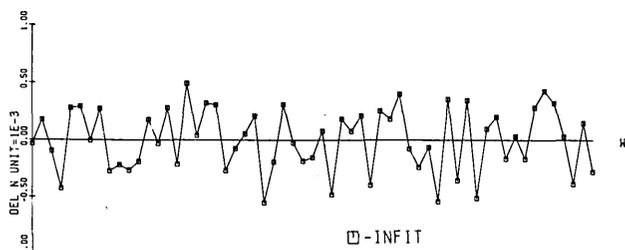


Fig. 3. Fitting error, zinc sulfide—fifty-nine points from 0.42 to 18.2 μm .

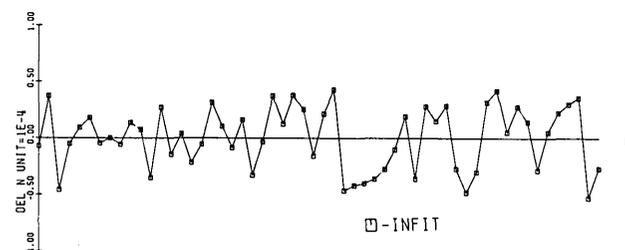


Fig. 4. Fitting error, zinc selenide—fifty-six points from 0.54 to 18.2 μm .

two fits for CsI is shown in Fig. 13.) Comparative results from the literature are also plotted where available. It is seen that our results and those obtained using the program described in Ref. 2 give equivalent results. As a matter of interest, the fitting of all the nonglass cases

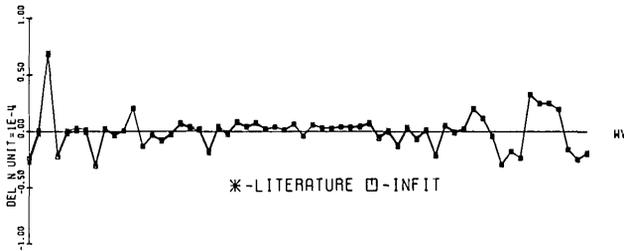


Fig. 5. Fitting error, fused silica—sixty points from 0.21 to 3.71 μm .

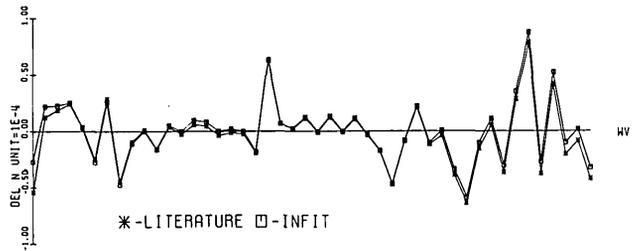


Fig. 10. Fitting error, sapphire—forty-six points from 0.27 to 5.58 μm .

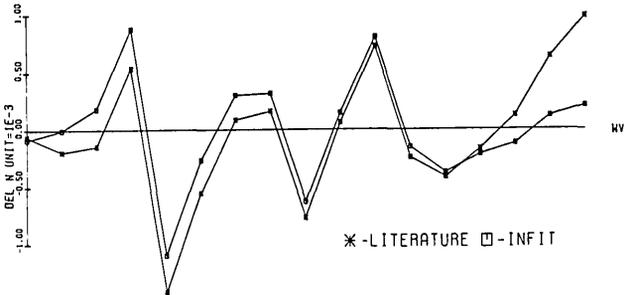


Fig. 6. Fitting error, germanium—seventeen points from 2.06 to 13.0 μm .

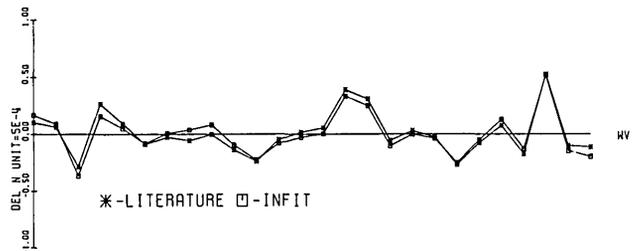


Fig. 11. Fitting error, arsenic trisulfide—twenty-six points from 0.58 to 11.9 μm .

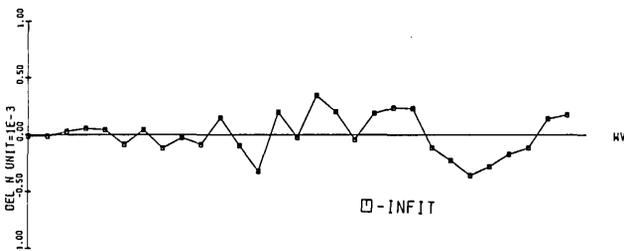


Fig. 7. Fitting error, silicon—thirty points from 1.36 to 11.0 μm .

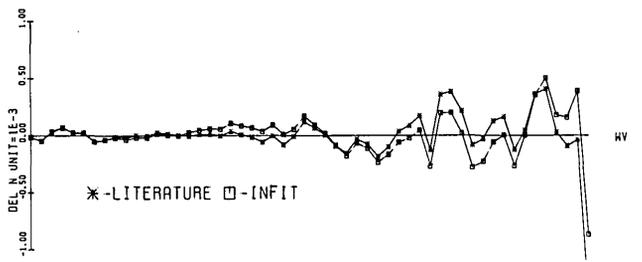


Fig. 12. Fitting error, cesium iodide—fifty-four points from 0.30 to 53.1 μm .

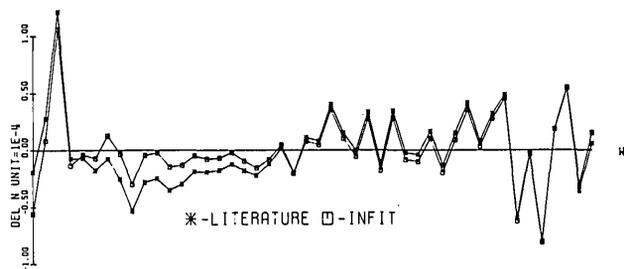


Fig. 8. Fitting error, fluorite—forty-six points from 0.23 to 9.72 μm .

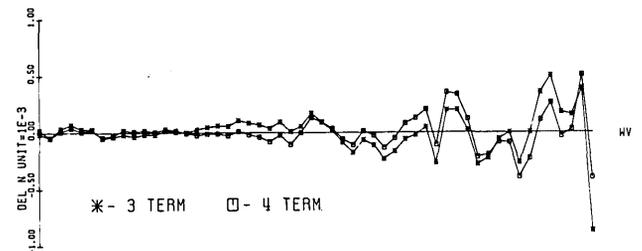


Fig. 13. Fitting error, cesium iodide—fifty-four points from 0.30 to 53.1 μm , three-term case vs four-term case.

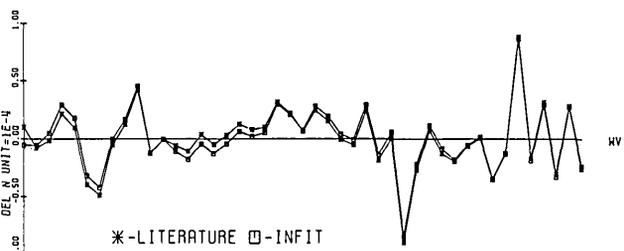


Fig. 9. Fitting error, barium fluoride—forty-five points from 0.27 to 10.3 μm .

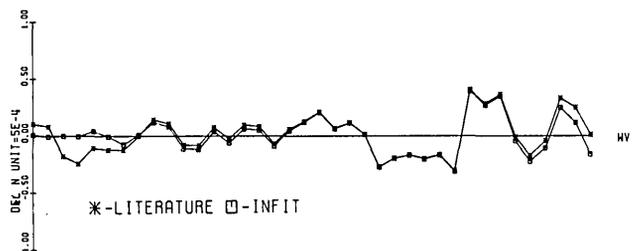


Fig. 14. Fitting error, thallium-bromide-iodide—thirty-eight points from 0.58 to 39.4 μm .

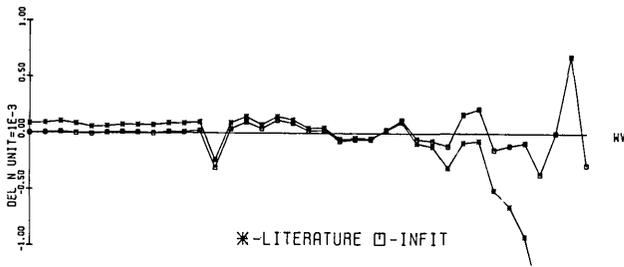


Fig. 15. Fitting error, cesium bromide—thirty-seven points from 0.37 to 39.2 μm .

mentioned, exclusive of the plotting, took less than 7 sec on a machine equivalent to an IBM model 68.

VI. Postscript

After the preceding pages were written, four other references on fitting refractive indices to the Sellmeier equation were discovered. Reference 21 is a compendium from many sources of optical and physical data for the alkali halides. Many separate measurements of index data are given for each material. These were obtained in different conditions including large differences of temperature, over different wavelength intervals, and with different accuracies, depending on the difficulty of the particular measurement. Some of the data extends well into the neighboring absorption bands of the transparent region. For each material, these data are combined into a single modified Sellmeier equation representing the dispersion of the material at 293 K. [The modification allows the constant term in Eq. (1) to be other than 1.] The resonance wavelengths [B_j in Eq. (1)] are obtained by physical measurements; a least-squares solution is used to obtain the A_j .

As a typical example taken from Ref. 21, we consider the material, cesium bromide. A six-term Sellmeier fit (five UV terms and one IR term) is given for this material covering the 0.21–55.0- μm band. For comparison, we fit the data in curve 1 on page 509 of Ref. 21, which gives index data for 37 wavelengths from 0.36 to 39.2 μm . These data were used because they seem to be the most accurate and cover most of the useful wavelength band of the material.

A four-term Sellmeier fit was obtained using INFIT (two UV terms, two IR terms). Figure 15 shows the results of this fit with that of the six-term fit from Ref. 21. The greater errors of the reference fit at both ends of the spectrum are undoubtedly due to the fact that that fit covers a greater bandwidth than considered here. However, the magnitude of the errors on the IR side seems to contradict the claimed accuracy of 1 in the fourth place. We attempted to readjust the numerator terms of the six-term Sellmeier fit given in Ref. 21 for the shorter range considered, but this failed because the six terms are not sufficiently independent over this range.

As a better test of INFIT's capability to fit this material in comparison to that of the six-term formula of the reference, we used the latter to generate forty-six index values evenly spread over the 0.25–40.0- μm range. This range was selected because it represents the useful range

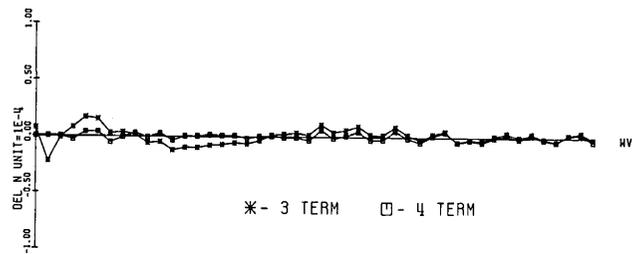


Fig. 16. Fitting error, cesium bromide—forty-six points from 0.25 to 40 μm generated by literature formula.

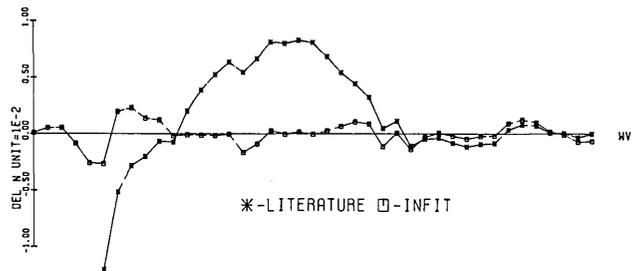


Fig. 17. Fitting error, cadmium sulfide O—forty-one points from 0.51 to 1.40 μm .

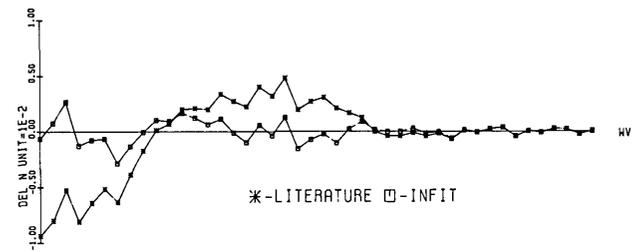


Fig. 18. Fitting error, cadmium sulfide E—forty-four points from 0.51 to 1.40 μm .

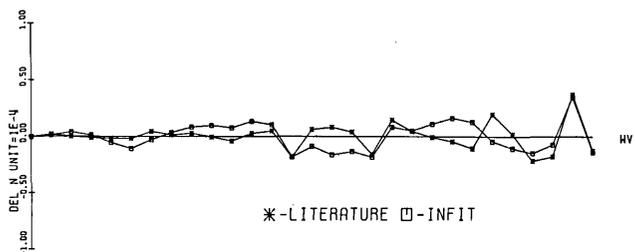


Fig. 19. Fitting error, zinc sulfide—twenty-nine points from 0.40 to 13.0 μm .

of the material for optical systems. Also, the accuracy of the index data available outside of this range is more than an order of magnitude less than that of the data within the range. Figure 16 shows how closely INFIT could fit these data with both a three- and four-term fit. The four-term fit consisted of three UV terms and one IR term. Both fits are well within the estimated uncertainty of the data used. Note that the error in Fig. 16 is plotted at a 10 \times scale relative to that of Fig. 15.

Reference 22 shows that a one-term Sellmeier equation can be transformed to a linear equation. Reference 23 extends this to show that an N -term Sellmeier

Table IV. Sellmeier Coefficients for Fits in Figs. 15 and 17-19

Material	A1	A2	A3	A4	A5
	B1	B2	B3	B4	B5
CsBr	8.84694025E - 01	9.01277636E - 01	9.91952400E - 02	2.70456187E + 03	
	8.37324633E - 02	1.65640698E - 01	5.87212331E + 01	3.92200000E + 03	
CdSO	3.96582820E + 00	1.81138737E - 01	-2.38694754E + 02		
	2.36228040E - 01	4.82851992E - 01	1.40000000E + 02		
CdSe	3.97478769E + 00	2.66808089E - 01	7.40772832E - 04	-3.22573381E + 01	
	2.24269842E - 01	4.66937848E - 01	5.09151386E - 01	9.89949494E + 01	
ZnS	7.92955926E - 01	3.06534624E + 00	2.44169740E - 01	8.40661571E - 01	2.04956238E + 03
	0.00000000E + 00	2.01416644E - 01	3.13426461E - 01	2.65551741E + 01	1.30000000E + 03

equation can be separated so that the denominator coefficients satisfy $N - 1$ simultaneous N th order equations. This method is already to be found for $N = 2$ in Ref. 1. It is pointed out there that this procedure is not equivalent to a least-squares fit to N because of the algebraic transformations. Reference 23 gives as an example a two-UV-term Sellmeier fit to the ordinary and extraordinary dispersions of single crystals of cadmium sulfide. Figures 17 and 18 show the fits obtained for both these cases from Ref. 23 compared with three-term fits using INFIT. Note that the missing term in the fits obtained in Ref. 23 is the IR term, whereas the greatest errors are on the UV side of the spectrum, indicating that the addition of an IR term probably would not result in a great improvement in the fit.

Reference 24 reports on new measurements of the index of chemical vapor grown zinc sulfide. These measurements represent an improvement in accuracy of more than an order of magnitude over the results in Ref. 10. The data were fit to a series whose terms are Chebyshev polynomials up to the eleventh order. The argument of the polynomials is the function of λ given by

$$x = [\log_e(\lambda - 0.25) - 0.3394896]/2.2060417.$$

The significance of this function, how the constants used in it were arrived at or how universal they are, is not explained.

Applying INFIT to these data proved to be a real test as it took a five-term Sellmeier formula to achieve a satisfactory fit. The results are shown in Fig. 19. This case is interesting because of the following two points. One is that the above formula seems to be a satisfactory alternative to using the Sellmeier formula. In fact, it seems to give a somewhat closer fit than the Sellmeier formula in the UV end of the spectrum. However, since both fits are within the claimed accuracy of the data, this may be due to the fact that the above series, being equivalent to a high-order polynomial, may just be following the errors closer. The other point is that our earlier remark that, based on our previous experience, a three-term Sellmeier fit was generally sufficient to satisfactorily fit the available data obviously has to be modified when the data become as accurate as in this case over a large wavelength range.

The coefficients of the Sellmeier fits to the four cases discussed in this section are given in Table IV.

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24. M. Debenham, "Refractive Indices of Zinc Sulfide in the 0.405–13- μ m Wavelength Range," *Appl. Opt.* **23**, 2238 (1984).
- 24–28 7th Int. Conf. on Laser Spectroscopy, Maui *T. Hansch, Physics Dept., Stanford U., Stanford, Calif. 94305*
- 24–29 Int. Conf. on Fourier & Computerized Infrared Spectroscopy, Ottawa *L. Baignee, Conf. Services Office, Ottawa, Ontario KIA 0R6, Canada*
- 25–27 11th Int. Symp. on Machine Processing of Remotely Sensed Data, West Lafayette *D. Morrison, Purdue U./LARS, 1291 Cumberland Ave., West Lafayette, Ind. 47906*

July

- 8–12 17th Int. Conf. on Phenomena in Ionized Glasses, Budapest *I. Abonyi Roland Eotvos Physical Soc., P.O. Box 240, 1368 Budapest, Hungary*
- 24–30 14th Int. Conf. on Physics of Electronics & Atomic Collisions, Palo Alto *SRI Int., 333 Ravenswood Ave., Menlo Park, Calif. 94025*
- 31–8 Aug. 17th Int. Congr. of History of Science, Berkeley *Congr. Secretariat, Off. for History of Science & Tech., 470 Stephens Hall, U. Calif., Berkeley, Calif. 94720*

August

- 4–8 Photoacoustic, Thermal & Related Sciences mtg., Quebec *L. Bertrand, Departement de genie physique, Ecole Polytechnique, Campus de l'Universite de Montreal, P.O. Box 6079, Succursale A, Montreal H3C 3A7, Canada*
- 18–23 29th Ann. Int. Tech. Symp. on Optical & Electro-Optical Eng., San Diego *SPIE, P.O. Box 10, Bellingham, Wash. 98227*
- 19–24 Int. Symp. on Lepton & Photon Interactions at High Energies, Kyoto *Res. Inst. for Fundamental Physics, Kyoto U., Oiwake-cho, Kita-shirakawa, Sakyo-ku, Kyoto 606 Japan*
- 19–30 23rd General Assembly of Inter. Assoc. of Semismology & Physics of the Earth's Interior, Tokyo *Intergroup Corp., Akasaka Yamakatsu Bldg., 8-5-32, Akasaka, Minato-ku, Tokyo 107 Japan*

September

- ? **Gradient-Index Optical Imaging Systems (Grin VI), Italy** *D. Moore, Inst. Optics, U. Rochester, Rochester, N.Y. 14627*
- 2–13 Laser Surface Treatment of Metals—NATO Advanced Study Inst., San Miniato *C. Draper, AT&T Tech., P.O. Box 900, Princeton, N.J. 08540*
- 9–12 Guided Optical Structures in the Military Environment Mtg., Ankara *V. Coyne, Surveillance Div., Rome Air Development Ctr./OCS, Griffis AFB, N.Y. 14331*
- 9–22 Niels Bohr Memorial Exhibition, Copenhagen Town Hall *AIP Bohr Library, 335 E. 45th St., New York, N.Y. 10017*

Meetings Calendar continued from page 4476

1985

May

- 6–8 3rd European Conf. on Integrated Optics, Berlin *I. Weber-Zuckarelli, Heinrich-Hertz-Institut Berlin GmbH, Bereich Integrierte Optik, Einsteinufer 37, D-1000 Berlin, FRG*
- 7–9 Basic Properties of Optical Materials Mtg., Wash., D.C. *A. Feldman, NBS, Bldg. 223, B-328, Wash., D.C., 20234*
- 12–16 38th Ann. Conf. SPSE, Atlantic City *W. Nebe, E.I. duPont de Nemours & Co., Inc., Experimental Station Bldg., 352, Rm. 155, Wilmington, Del. 19898*
- 19–24 2nd U.S. - Dutch Int. Symp.: Aerosols, Williamsburg *S. Lee, U.S. Coordinator, U.S. Environmental Protection Agency, Res. Triangle Park, N.C. 27711*
- 21–24 **OSA/IEEE Lasers & Electro-Optics Conf.**, Baltimore *OSA Mtgs. Dept., 1816 Jefferson Pl., N.W., Wash., D.C. 20036*

June

- 9–13 Soc. for Experimental Stress Analysis Spring Mtg., Las Vegas *SESA, 14 Fairfield Dr., Brookfield Ctr., Conn. 06805*
- 10–13 **Int. Lens Design, OSA Tech. Mtg.**, Cherry Hill *OSA Mtgs. Dept., 1816 Jefferson Pl., N.W., Wash., D.C. 20036*
- 10–14 **OSA Spring Conf.**, Cherry Hill *OSA Mtgs. Dept., 1816 Jefferson Pl., N.W., Wash., D.C. 20036*
- 10–14 Image Science & Technology ICO Conf., Helsinki *P. Oittinen, Helsinki U. Technology, Lab. of Graphic Arts Tech., Tekniikantie 3, 02150 Espoo 15, Finland*
- 12–14 **Workshop on Optical Fabrication & Testing, OSA Tech. Mtg.**, Cherry Hill *OSA Mtgs. Dept., 1816 Jefferson Pl., N.W., Wash., D.C. 20036*
- 17–19 Int. Conf. on Chemical Kinetics, Gaithersburg *J. Heron, A147 Chem. Bldg., NBS, Wash., D.C. 20234*

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