

ON ERRORS OF REFLECTIVITY MEASUREMENTS AND  
OF CALCULATIONS OF REFRACTIVE INDEX  $n$   
AND ABSORPTION COEFFICIENT  $k$

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ABSTRACT

First, the sources of errors are discussed which arise from the condition of specimen and equipment in reflectivity measurements with a microscope using vertically incident light. Although ways of increasing the accuracy can be given, it appears that relative errors of about  $\pm 0.5\%$  to  $\pm 1\%$  are unavoidable even under most favorable conditions. It is then shown that errors of reflectivity values in air and oil strongly affect the accuracy of refractive indices  $n$  and absorption coefficients  $k$  calculated therefrom by means of Beer's equation. This is demonstrated for assumed relative errors of  $\pm 1\%$  and of  $\pm 5\%$  of the reflectivity in air and/or oil by the calculated relative errors of  $n$  and  $k$  which vary considerably in  $n$ - $k$  plots. The characteristics of three different types of  $\Delta n/n$  and  $\Delta k/k$  diagrams are discussed and equations for the exact determination of these errors given.

INTRODUCTION

In recent years the devices for quantitative measurements in reflected light have been improved considerably. It is true that there are still numerous sources of errors but the errors caused by the apparatus have been decreased to such an extent that it now appears possible to measure reflectivity reliably. Cameron (1961) has developed methods of another kind (measurement of rotation properties, etc.) based on papers by earlier authors, especially by Berek (1931). All this has led to an increased interest in reflected-light microscopy, especially with polarized light, and it may be said that the quantitative stage is now being approached which was achieved about 50 years ago in transmitted-light microscopy.

Nevertheless, it should be realized that in all measurements in reflected light the sources of errors and their effects on the results are normally considerably larger than in transmitted light. The present paper deals with the problems involved in the determination of reflectivities and the calculation of optical constants therefrom. *Reflectivity* remains the most important optical property of a reflecting surface. Reflectivity values have already been compiled in several books on ore minerals, and recently Bowie and Taylor (1958) have developed a system of ore mineral identification from two quantitative values: reflectivity and micro-hardness. Cambon (1947) has shown in a comprehensive paper that reflectivity measurements are useful also for investigations of metals and alloys. Koritnig (1963) has made a successful attempt to correlate the reflectivity of mix-crystals with their chemical composition.

Apart from these applications, it is also interesting to trace the reflectivity back to more fundamental values such as refractive index  $n$  and absorption coefficient  $k$  (or absorption index  $\kappa = k/n$ ) because these are of special importance in crystal physics. The value  $k$  represents the decrease of the amplitude of a homogeneous wave  $A_0$  in the reflecting material over a distance equal to the wavelength of the light in vacuum  $\lambda_v$ :

$$A_{\lambda v} = A_0 \cdot e^{-2\pi k} \quad (1)$$

The values  $n$  and  $k$  can be calculated from the reflectivity measured in two different immersion media. The necessary equations are obtained by inverting Beer's relation for the reflectivity

$$R_i = \frac{(n - n_i)^2 + k^2}{(n + n_i)^2 + k^2} \quad (2)$$

where  $n$  is the refractive index of the reflecting material and  $n_i$  that of the immersion medium. The media air ( $n_i = n_0 = 1$ ) and immersion oil ( $n_i = n_1 \approx 1.515$ ) are used in practical work. With the reflectivities  $R_0$  and  $R_1$  measured in these two media, the equations for  $n$  and  $k$  are as follows:

$$n = \frac{0.5 \cdot (n_1^2 - 1) \cdot (1 - R_0) \cdot (1 - R_1)}{n_1 \cdot (1 - R_0)(1 + R_1) - (1 + R_0)(1 - R_1)} \quad (3)$$

$$k = \sqrt{\frac{2 \cdot n_1}{n} \cdot \frac{1 + R_1}{1 - R_1} - \left(1 + \frac{n_1^2}{n^2}\right)} = \sqrt{\frac{2}{n} \cdot \frac{1 + R_0}{1 - R_0} - \left(1 + \frac{1}{n^2}\right)} \quad (4)$$

These equations are given in another transformed way by Berek (1953, p. 331, after Königsberger). Nomograms for a graphical evaluation of  $n$  and  $\kappa$  ( $= k/n$ ) were published by Volynskii and Yasnopol'skii (1959).

In reflectivity measurements, there are *errors* caused by the equipment and its operation and also errors caused by the specimen. In calculations of  $n$  and  $k$  from  $R_0$  and  $R_1$ , the error limits are changed by the mathematical treatment.

#### ERRORS CAUSED BY THE EQUIPMENT

Since the first photometric measurements of reflectivity under the microscope by Orcel (1927) and Berek (1931), much experience has been gained, and several special types of equipment have been described. The modern standard equipment includes the following elements: light source, monochromator, reflected light microscope, light detector, amplifier, and indicating device. The single-beam photometer with photocell or electron multiplier is now regarded as the most efficient kind of apparatus for this work.

##### 1. *Errors caused by the mechanical properties of the microscope*

The microscope and all parts connected with it must have outstanding mechanical stability, because the photo-electric equipment is rather sen-

sitive to vibrations. During the measurement, care should be taken to avoid the slightest movement of the microscope when the filter slides or the polarizers or other devices are handled or the microscope stage is rotated. The errors caused by lack of mechanical stability increase with the magnification used.

As an example, a series of reflectivity measurements with the specimen defocussed by  $1 \mu\text{m}^1$  gave the deviations in Table 1 from the values measured at exact focus.

2. Errors caused by the optical properties of the microscope

Sources of error of this kind are scattered light and reflections and also beam deflection by optical elements which are out of adjustment.

TABLE 1. INFLUENCE OF DEFOCUSING BY  $1 \mu\text{M}$  ON REFLECTIVITY VALUES

Objective	Magnification	Approx. depth of focus after Michel (1957) given in $\mu\text{m}$	Relative change of indication given in % at "extra-focal adjustment" by $1 \mu\text{m}$
2.5/0.08	25:1	150	$5 \times 10^{-4} \%$
6.3/0.16	63:1	28	$5 \times 10^{-3} \%$
16/0.32	160:1	5	$3.5 \times 10^{-2} \%$
40/0.85	400:1	1	0.15%
100/1.25 oil	1000:1	0.3	0.5%

Scattered light and reflections occur at glass/air surfaces, at cemented surfaces of lenses or at light filters, lens mountings, and inner tube walls. Careful "blooming" and correct arrangement of a sufficient number of diaphragms by the manufacturer and the correct use of iris diaphragms by the observer (e.g. strict observance of the Köhler principle of illumination) are absolutely necessary.

The objective lenses may often have detrimental effects. Reflex images of the light source which overlap the image of the object may arise unavoidably in the central parts of the objectives. This effect can be eliminated by almost closing the field and aperture diaphragm and especially by using slightly *oblique* illumination. For this purpose a trapezoid prism reflector as suggested by Berek (1931) is of special advantage. Compared with a plane-glass reflector a greater percentage of the entering beam is reflected onto the specimen.

On the other hand, the inclination of the incident light should not be

<sup>1</sup>  $1 \text{ mm} = 10^3 \mu\text{m} = 10^6 \text{ nm}$ .

too large; in particular the aperture of the light cone (numerical aperture of the illumination) should be kept small so that the illumination can still be considered as vertical. Even when high power objectives are used, the inclination can be nearly vertical if the aperture diaphragm is closed as far as possible. Consequently, a movable aperture diaphragm is of utmost importance.

Finally, disturbing reflections can even occur at the plane surfaces of glass filters between light source and object. These reflections can be eliminated by slightly tilting the filters.

### 3. *Errors caused by the properties and the operation of the supplementary devices*

The stabilization of the current for the light source is as highly important as it is for the light detector and for the amplifier with the indicating device. In instruments of maximum sensitivity, the temperature influence must be considered. It can be eliminated by an extended response time and constant room temperature. The fatigue of the light detector and its varying spectral sensitivity can be balanced by using suitable types of detectors. Photo-multiplier tubes should be used and it has been found most satisfactory to select the most stable ones from types manufactured in large quantities. Experience shows that there are usually rather large differences in properties and in quality, even in tubes of the same type.

The higher the dispersion of reflectivity of the object, the stronger are the extremely complex effects of the properties, dependent on wave length, of the different optical elements on the accuracy of the measurement. Among these the spectral characteristics of the detector and especially those of the color filter (Bowie 1962), as well as that of the light source, are of decisive importance. To make results obtained by different observers comparable, light as strictly monochromatic as possible should be used. In view of all the difficulties involved it cannot be recommended to use "white" light (Ramdohr 1963)! Each paper on reflectivity measurements should contain a graph giving the spectral sensitivity of the equipment used. It is advisable to select standard wavelengths; among these, especially  $\lambda = 546$  nm has been discussed by the Commission on Ore Microscopy of the International Mineralogical Association (I.M.A.).

In reflectivity measurements in oil, reflected and scattered light effects generally have a stronger influence on the results than in air (Piller 1959). They have either to be eliminated very carefully or taken into consideration as correction factors. In order to guarantee reproducible results all laboratories should use oil of equal quality (*e.g.*, immersion oil of paraffin type with  $n_i = 1.515$  at  $\lambda = 589$  nm and  $20^\circ$  C.) with low dispersion of  $n_i$  and only small change of  $n_i$  with temperature (these variations must be

known for calculations of  $n$  and  $k$ , see page 873). The microscope objective must be designed in such a way that it can be used as an immersion objective. Objectives of lower magnification can be provided with "immersion caps," whereas objectives of higher magnification have to be specially computed.

#### ERRORS CAUSED BY THE SPECIMEN

An important source of error in reflectivity measurements is the surface condition of the specimen. In the last decades considerable progress has been made in preparing suitable polished surfaces (see, for example, Schneiderhöhn 1952 and further improvements *e.g.* by Rehwald 1952 and Hallimond 1963), especially through the use of diamond as the grinding and polishing material. Comparison measurements of reflectivity after different ways of polishing have, for example, been made by Cissarz (1932). Nevertheless, there is still a need for a method for determining the quality of a surface which would be necessary for a comparison of the results of different investigators. Work in this direction has been started by W. Uytendogaardt (personal communication).

The surface of the object has to be sufficiently large (depending on the sensitivity of the measuring device) and homogeneous, carefully polished, and completely free from relief. In substances of low absorption coefficient, centers of scattered light (internal reflections) beneath the surface may be disturbingly noticeable, especially when they are within or near the depth of the focus range (Table 1).

Furthermore, the reflecting surface has to be exactly perpendicular to the microscope axis so that the direction of light propagation and the geometry of the light rays remain absolutely constant when standard and specimen are exchanged, when the specimen is moved, or when the microscope stage is rotated. According to the experience of the authors even very small changes in the geometrical conditions of the light propagation have a considerable influence on the measured reflectivities. The correct alignment should be checked by looking at the upper focal plane of the objective, *e.g.* with a Bertrand lens; the image of the condenser aperture diaphragm should not move upon rotation of the microscope stage.

For the comparison standard the same considerations are valid. Its reflectivity should be measured under exactly the same conditions as that of the object. In order to increase the accuracy of the results, a series of standards of different reflectivities should be used.

#### FUNDAMENTAL ERRORS IN CALCULATIONS OF $n$ AND $k$ FROM $R_0$ AND $R_1$

The previous chapters indicate that reflectivity measurements are subject to errors which cannot be neglected. According to the experience of the authors these are normally between  $\pm 1$  and  $\pm 5$  relative per cent. In

cases of high reflectivity the relative error may be as low as  $\pm 0.5\%$  while in cases of very low reflectivity it may even rise to  $\pm 10\%$ . A good accuracy which can sometimes be reached would be  $\pm 1\%$ ; therefore, the following calculations are carried out for this error, and some supplementary data are given for errors of  $\pm 5\%$ .

The errors assumed here may be considered too high. But it has to be kept in mind that the errors given normally in papers on reflectivities are only *reproducibilities* for a given set of equipment. They do not include fundamental errors introduced by specimen or equipment.

For some purposes it is sufficient if this reproducibility is known. An example is the determination of optical symmetry from reflectivity measurements after Cameron (1963) who obtained an accuracy of the absolute values of  $\pm 0.2\%$  (corresponding to a relative error of  $\pm 1$  per cent at a reflectivity of  $0.20 = 20\%$ ).

When reflectivities are to be used as constants or as starting values for calculations of  $n$  and  $k$ , however, the *real* errors have to be considered. They are, of course, larger than the reproducibilities of single instruments and can be obtained from data collected on identical specimens in different laboratories with different types of equipment. Comparative measurements of this kind have still to be made.

What is the effect of these errors in reflectivity on the calculated values of  $n$  and  $k$ ? Wright (1919) has stated, without giving quantitative data on errors, that  $n$  and  $k$  cannot be calculated with sufficient accuracy from reflectivity measurements. Some more detailed information on this subject can be derived for special cases from Cambon's (1947) paper, but until now the quantitative effects of errors in reflectivity on the accuracy of the calculated values have not been treated generally.

To begin with, the ideal relations are shown in Fig. 1. Here it has been assumed that no error occurs. Physically, only such combinations of  $R_0$  and  $R_1$  are possible which lie within the "cigar"-shaped field. Only a single pair of  $n$  and  $k$  corresponds to each pair of  $R_0$  and  $R_1$ . Every error in  $R_0$  and/or  $R_1$  normally leads to erroneous values both of  $n$  and  $k$ .

A figure similar to Fig. 1 has already been given by Ponomareva (1958)<sup>1</sup> who found that nearly all solid substances have their representative points or areas in the lower right half of the "cigar" bordered by the diagonal (furthermore, minerals with certain types of bonding occupy special areas within the distribution). This means that the reflectivity in oil is normally lower than in air. Exceptions to this rule occur if the refractive index  $n$  of the mineral is closer to  $n_{\text{air}}$  than to  $n_{\text{oil}}$  (see equation (2)); for example, Gehlen and Piller (1964) found the reflectivity of  $\omega$  of covellite to be slightly higher in oil than in air for red light.

<sup>1</sup> The authors would like to thank Dr. A. H. van der Veen, Metallurgical Research Lab., N.V. H.M.B., Arnhem (Netherlands), for having drawn their attention to this paper.

But not only errors in reflectivity affect the calculated values of  $n$  and  $k$ . Errors are also introduced when the dispersion of  $n_1$ , that is, of the refractive index of the immersion oil, is neglected in equations (3) and (4). For example, using the average value of  $n_1 = 1.515$  instead of the correct one of 1.5223 at  $\lambda = 486$  nm would have led to a relative error of 24% in the calculated  $k_e$  of covellite (according to data by Gehlen and Piller 1964). An error of this kind would be negligible near  $\lambda = 589$  nm but could

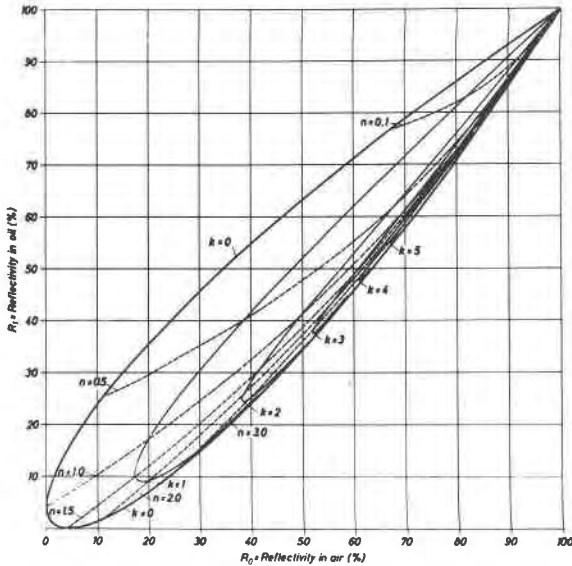


FIG. 1. Relations between reflectivity  $R_0$  in air ( $n_0 = 1.000$ ), reflectivity  $R_1$  in oil ( $n_1 = 1.515$ ), refractive index  $n$  (dashed curves), and absorption coefficient  $k$  (solid curves), calculated from Beer's equation for vertically incident light (2).

be large in extreme parts of the visible spectrum. This error is not considered further.

In the following discussion we shall use the expressions  $\Delta n = n^* - n$ ,  $\Delta k = k^* - k$ ,  $\Delta R_0 = R_0^* - R_0$ , and  $\Delta R_1 = R_1^* - R_1$  where  $R_0$ ,  $R_1$ ,  $n$ , and  $k$  are the correct values while  $R_0^*$  and  $R_1^*$  are the assumed measured values (normally erroneous) and  $n^*$  and  $k^*$  the erroneous constants derived therefrom. For example,  $R_1^* = 1.01 R_1$  means that the reflectivity in oil has been assumed to be measured too highly by 1%, while in  $R_0^* = R_0$  it has been assumed that the air value was correct.

In order to draw a graph of the errors  $\Delta n/n$  and  $\Delta k/k$  which both are functions of  $n = f(R_0, R_1)$ ,  $k = f(R_0, R_1)$ ,  $\Delta R_0/R_0$ , and  $\Delta R_1/R_1$ , many calculations are necessary since simplified approximating equations cannot be applied.

The following equations have been used (with  $n_0=1.0$  and  $n_1$  kept constant at 1.515):

$$\frac{n^* - n}{n} = \frac{\Delta n}{n} = \frac{n_1 \cdot \frac{1 + R_1}{1 - R_1} - n_0 \cdot \frac{1 + R_0}{1 - R_0}}{n_1 \cdot \frac{1 + R_1^*}{1 - R_1^*} - n_0 \cdot \frac{1 + R_0^*}{1 - R_0^*}} - 1 \quad (5)$$

$$\frac{k^* - k}{k} = \frac{\Delta k}{k} = \sqrt{\frac{\left(\frac{2 \cdot n_0}{1 - R_0^*}\right)^2 \cdot R_0^* - \left\{ \frac{0.5 \cdot (n_1^2 - n_0^2)}{n_1 \cdot \frac{1 + R_1^*}{1 - R_1^*} - n_0 \cdot \frac{1 + R_0^*}{1 - R_0^*}} - \frac{1 + R_0^*}{1 - R_0^*} \right\}^2}{\left(\frac{2 \cdot n_0}{1 - R_0}\right)^2 \cdot R_0 - \left\{ \frac{0.5 \cdot (n_1^2 - n_0^2)}{n_1 \cdot \frac{1 + R_1}{1 - R_1} - n_0 \cdot \frac{1 + R_0}{1 - R_0}} - \frac{1 + R_0}{1 - R_0} \right\}^2}} - 1 \quad (6)$$

The calculating time has been reduced by means of a computer and by using narrowly graded pairs of  $n$  and  $k$  (or  $R_0$  and  $R_1$ ) and errors of measurement of  $\pm 1\%$  and  $\pm 5\%$ . The results have been analyzed graphically by plotting curves which connect equal errors  $\Delta n/n$  and  $\Delta k/k$ . All 16 assumptions listed in Table 2 have been investigated.

Figure 2 gives the errors for assumption 2 in a  $R_0/R_1$  diagram comparable with Fig. 1. The relations are more clearly seen in  $n/k$  diagrams. The

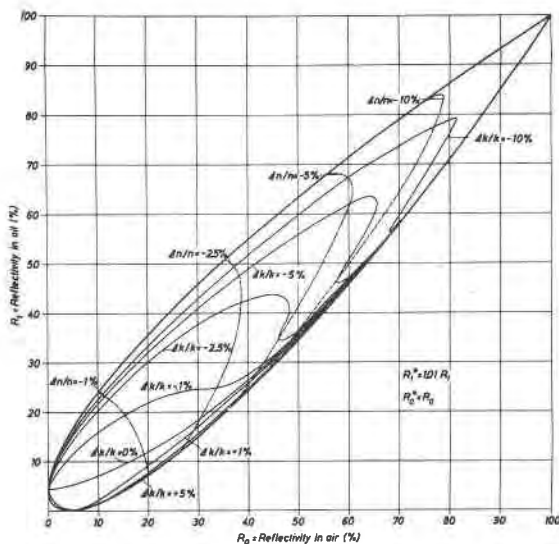


FIG. 2. Relative errors  $\Delta n/n$  (dashed curves) and  $\Delta k/k$  (solid curves) in a  $R_0/R_1$  diagram similar to Fig. 1, calculated under the assumption that the measured reflectivity in air ( $R_0^*$ ) is correct while in oil ( $R_1^*$ ) it has been measured too high by 1 rel. per cent (case 2, Table 2).



TABLE 2. GENERAL CHARACTERISTICS OF THE CURVES OF EQUAL ERROR  $\Delta n/n$  AND  $\Delta k/k$  IN A SYSTEM OF  $n/k$  COORDINATES

Number of assumption	Fig. in which type is shown	Assumption		$\Delta n/n$ curves			$\Delta k/k$ curves			
		Relation between the assumed correct reflectivity values $R_0$ in air and $R_1$ in oil and the assumed incorrect $R_0^*$ and $R_1^*$	Sign of error	Coordinates $n$ and $k$ of the smallest error	Amount of the smallest error (%)	General characteristics of the error with respect to the coordinates $n$ and $k$	Sign of error	Significant $n/k$ pairs for the main curve of smallest error ( $\Delta k/k \approx 0\%$ ) (second pair only valid for assumptions 1 through 8)	Values of $n$ at which all $\Delta k/k$ curves concur near the abscissa <sup>2</sup>	
1 (9)	4	$R_0^* = 1.01 R_0$ $R_1^* = R_1$ $(R_0^* = 1.05 R_0)$ $(R_1^* = R_1)$	+	$n = 1$ $k = 0$	0		+ -	$n = 1.515$ about 2	near 0 about 5	1.515
2 (10)	3	$R_0^* = R_0$ $R_1^* = 1.01 R_1$ $(R_0^* = R_0)$ $(R_1^* = 1.05 R_1)$	-	$n = 1.515$ $k = 0$	0		- +	$n = 1$ 5	near 0 about 4	1.0
3 (11)	3	$R_0^* = 0.99 R_0$ $R_1^* = R_1$ $(R_0^* = 0.95 R_0)$ $(R_1^* = R_1)$	-	$n = 1$ $k = 0$	0		- +	$n = 1.515$ 5	near 0 about 3.5	1.515
4 (12)	4	$R_0^* = R_0$ $R_1^* = 0.99 R_1$ $(R_0^* = R_0)$ $(R_1^* = 0.95 R_1)$	+	$n = 1.515$ $k = 0$	0	The error grows considerably at $n < 0.5$ and $n > 5$ and $k > 1.5$	+ -	$n = 1$ about 2.5	near 0 5	1.0
5 (13)	5	$R_0^* = 1.01 R_0$ $R_1^* = 1.01 R_1$ $(R_0^* = 1.05 R_0)$ $(R_1^* = 1.05 R_1)$	+ -	$n \leq \sqrt{1.515}$ $k < 2$	0		+ -	$n = 1.515$ about 4.5	near 0 5	1.515 1.0
6 (14)	4	$R_0^* = 1.01 R_0$ $R_1^* = 0.99 R_1$ $(R_0^* = 1.05 R_0)$ $(R_1^* = 0.95 R_1)$	+	$n = \sqrt{1.515}$ $k = 0$	about 0.1		+ -	$n = 1$ about 2	near 0 about 4	$\sqrt{1.515}$ 1.515
7 (15)	3	$R_0^* = 0.99 R_0$ $R_1^* = 1.01 R_1$ $(R_0^* = 0.95 R_0)$ $(R_1^* = 1.05 R_1)$	-	$n = \sqrt{1.515}$ $k = 0$	about 0.1		- +	$n = 1$ 5	near 0 about 3.5	1.0 $\sqrt{1.515}$ 1.515
8 (16)	5	$R_0^* = 0.99 R_0$ $R_1^* = 0.99 R_1$ $(R_0^* = 0.95 R_0)$ $(R_1^* = 0.95 R_1)$	- +	$n \leq \sqrt{1.515}$ $k < 2.5$	0		- +	$n = 1.515$ 5	near 0 about 4	1.515 1.0

<sup>1</sup> For assumptions 5 through 8 there exists a second smaller ( $\Delta k/k = 0$ ) curve.  
<sup>2</sup> For assumptions 6 and 7 only part of the curves are concurring.

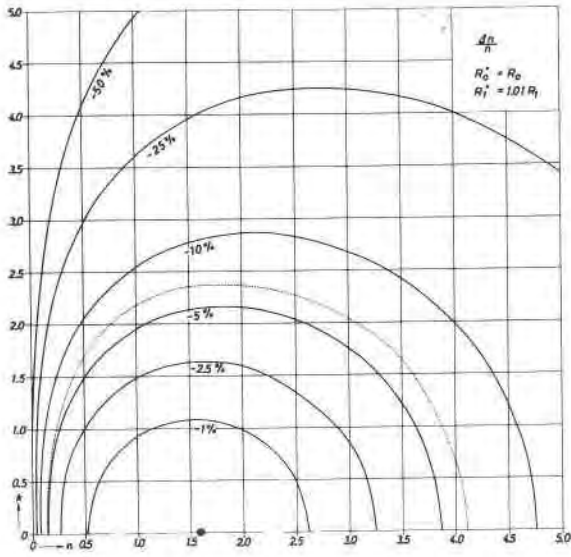
results obtained under the various assumptions (Table 2) can be grouped in three different types of error diagrams. In each of these the error curves have similar shapes; only the distances between corresponding error curves are different in single cases belonging to the same type. Figures 3a and 3b (case 2) give an example of the first type (cases 2, 3 and 7 and corresponding 5% cases), Figs. 4a and 4b (case 6) one of the second type (cases 1, 4 and 6 etc.), and Figs. 5a and 5b (case 8) one of the third type (cases 5 and 8 etc.). The dotted lines in these figures indicate the position of selected curves from the corresponding 5% error diagrams. The specific characteristics of each case are summarized in Table 2.

In Figs. 4 a, b, the shaded fields indicate the areas where in all 1% cases the errors  $\Delta n/n$  resp.  $\Delta k/k$  are  $\leq |5|%$ . With the exception of small parts derived from cases 7 and 5 (for  $\Delta k/k$ ), these fields are bordered by the 5% curves of case 6 (Figs. 4a and 4b) which turns out as the most unfavorable one.

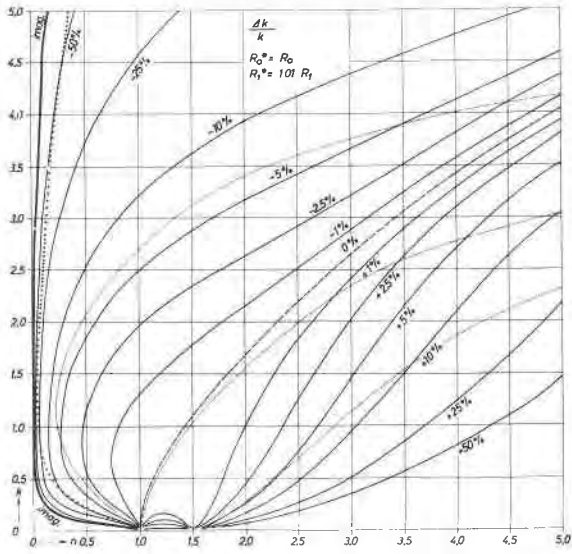
## RESULTS

Errors in reflectivity values have a very complex effect on the accuracy of the calculated constants  $n$  and  $k$ . For these the relative error is generally much larger than that of the measured reflectivities. Only  $n$  and  $k$  values within the hatched areas of Figs. 4 a, b can be determined with sufficient reliability since their error does not exceed  $\pm 5%$  provided the errors of measurement of both reflectivities do not exceed  $\pm 1%$ . Outside these areas the errors of  $n$  and  $k$  are normally inacceptably large. There are only certain combinations of  $n$  and  $k$  outside the hatched areas where  $\Delta k/k$  is small or even zero. If such a case can be expected the error must be calculated by means of equations (5) and (6) from the errors in  $R_0$  and  $R_1$  which have been ascertained experimentally.

Consequently, there are numerous cases, especially when substances of very low or very high  $n$  and/or very large or partly also very low  $k$  are investigated, where  $n$  and especially  $k$  cannot be determined with sufficient accuracy from reflectivity measurements. There is even a danger that negative refractive indices or imaginary absorption coefficients might be calculated (as was recently done in a few cases by Kaemmel, 1962) which must be attributed to errors in reflectivity measurements. The limits of the imaginary fields in the  $\Delta k/k$  plots which are given by  $k^*=0$ ;  $\Delta k/k = -100%$  are shown in Fig. 6 for cases 1 through 8 (Table 2). The most unfavorable case is marked 1-8 (lower right hand corner of Fig. 6). This case means that for every combination of  $n$  and  $k$  outside this hatched area even an error of only  $\pm 1%$  of the reflectivity values can lead to imaginary values of  $k$ , *i.e.*, the erroneous  $R_0^*/R_1^*$  pairs have representative points outside the "cigar"-shaped area in Fig. 1 and are therefore unreal.



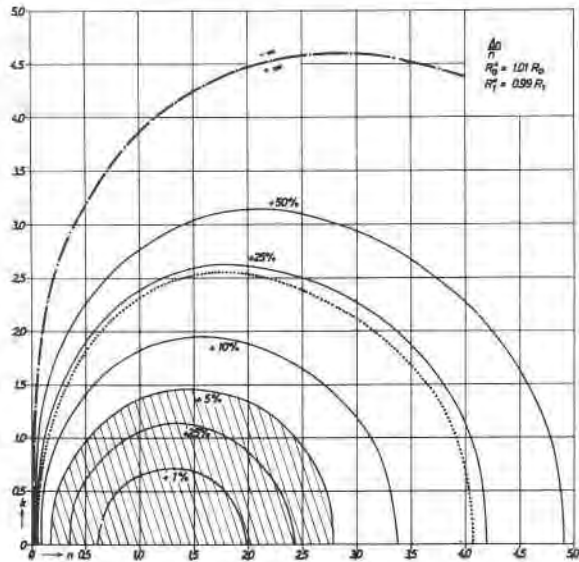
(a)



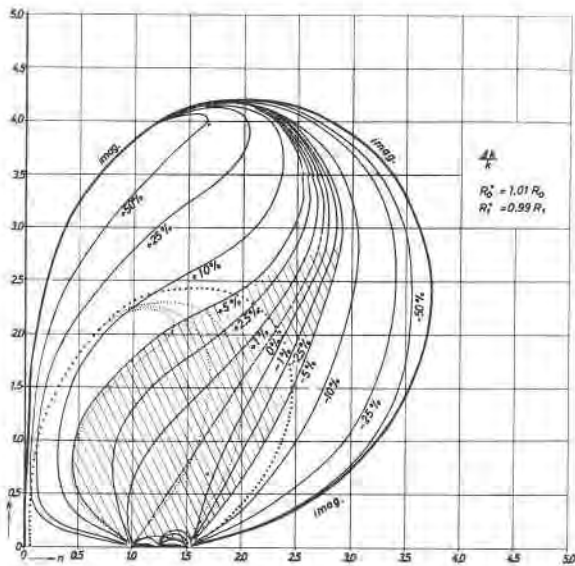
(b)

FIGS. 3-5. Relations between refractive index  $n$ , absorption coefficient  $k$ , and relative error  $\Delta n/n$  (a) resp.  $\Delta k/k$  (b), calculated as described in the text under three of the assumptions listed in Table 2. Solid lines=1% error in reflectivity value(s) assumed; dotted lines=5%.

FIGS. 3a and b. Assumption 2 (Table 2). Dotted line in Fig. 3a: -25%, assumption 10. Dotted lines in Fig. 3b from upper left to lower right: limit of the imaginary field, -25%, 0%, and +25%, assumption 10.

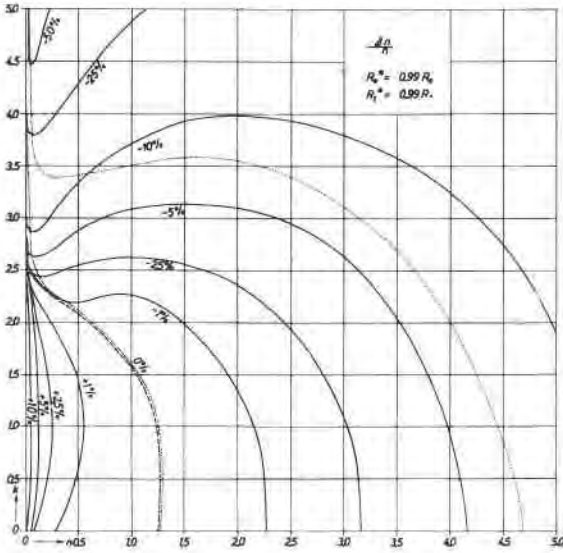


(a)

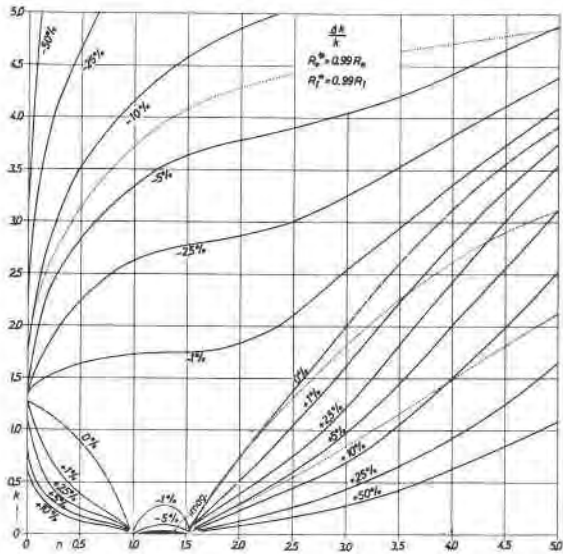


(b)

FIGS. 4a and b. Assumption 6 (Table 2). Dotted line in Fig. 4a:  $-\infty/+\infty$  limit, assumption 14. Dotted lines in Fig. 4b: heavy dots, limit of the imaginary field; small dots, from left to right, +25%, 0%, and -25%, assumption 14. Hatched areas: fields of errors  $\leq |5|%$  for the most unfavorable case from assumptions 1 through 8.



(a)



(b)

FIGS. 5a and b. Assumption 8 (Table 2). Dotted lines in Fig. 5a from left to right: 0%, -25%, assumption 16. Dotted lines in Fig. 5b from upper left to lower right: -25%, 0%, and +25%, assumption 16.

But even in less critical  $n/k$  areas the errors of  $n$  and  $k$  increase considerably with errors in  $R_0$  and  $R_1$ . Therefore, greatest care has to be taken in reflectivity measurements that a device of highest quality is used and operated correctly. Methods and instruments for determining reflectivity should be standardized as much as possible, and the error limit of each value should be given.

Sometimes the accuracy of  $R$ ,  $n$ , and  $k$  values can be increased in an additional way: Gehlen and Piller (1964) not only determined the reflec-

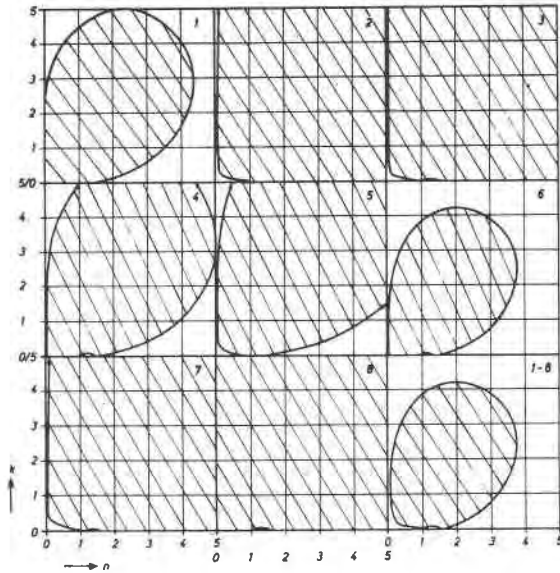


FIG. 6. Composite  $n/k$  graph of the limits of the imaginary fields (not hatched) of errors  $\Delta k/k$  (curves  $\Delta k/k = -100\%$ ) for assumptions 1 through 8 (Table 2). 1-8 is the most unfavorable case constructed therefrom.

tivities of covellite at several different wavelengths but also in several oriented sections through single crystals. Construction of dispersion curves permitted checks and minor corrections of single values, while reasonable extrapolations of  $n$  or  $k$  versus orientation curves (from regions of higher accuracy into regions of low accuracy) helped to determine the  $\epsilon$  values which otherwise would have been very inaccurate.

Therefore, determinations of optical data in reflected light should not be made at single wavelengths only but at a series of them in order to make checks and extrapolations possible. Further, in anisotropic minerals the crystal orientation should be known before  $n$  and  $k$  values are derived.

In all cases where reflectivities are measured or especially where  $n$  and  $k$  values are calculated from them, a discussion of errors is absolutely necessary.

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