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Surface Radiation Properties of ThO_2 and Other Reactor Materials

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ABSTRACT

This technical report summaries the results obtained on surface radiation properties of ThO_2 and other related reactor materials. The content herein is based on the M.S. dissertation submitted by H.H. Ma, Department of Mechanical Engineering, University of Wisconsin at Milwaukee, December 1979. It is compliment to the previous report - CDO-4040-3, 1978, which summaries the results of UO_2 and other pertaining materials.

Specifically, the present study provides surface radiation properties of three nuclear reactor materials; thorium dioxide, sodium and steel (99 Fe + 1 C). First, based on transmission spectra and Kramers-Kronig analysis, the complex refractive index, which is fundamental to surface radiation property calculations, of ThO_2 is presented over a wide spectral range. Then depending on the contacting media, three types of the surfaces are considered. They are the interfaces between ThO_2 and Sodium, ThO_2 and Steel (99 Fe + 1 C) as well as ThO_2 and a gas. For each interface, the spectral interface reflectance from one side of the medium to the other side is evaluated for all wavelengths. These spectral properties are further integrated to yield the total hemispherical properties over a temperature range, 1200°K to 6000°K, of interest to reactor safety analysis.

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NOMENCLATURE

I - intensity of radiative flux

k - extinction coefficient

$K_{a\lambda}$ - absorption coefficient

n - real index of refraction

$\hat{n}$ - complex index of refraction ($= n - ik$)

T - temperature

Greek:

α - total absorptance

α_λ - spectral absorptance

ε - total emittance

ε_λ - spectral emittance

ϕ - phase angle

θ - incidence angle

λ - wavelength

ρ - total reflectance

ρ_λ -spectral reflectance

Subscripts:

1 - medium 1

2 - medium 2

i - incident quantity

n - normal direction

s -source

t - transmitting quantity

λ - wavelength

I. INTRODUCTION

In the safety analysis of nuclear reactors, the temperature of the reactor materials involved often is high enough (1200 to 6000°K) that thermal radiative transfer may become an important mode of heat transfer as compared to conduction and convection.[1-4] To perform radiative transfer calculations, the information on thermal radiation properties of reactor materials is needed. Chan and Tseng[5] recently presented the surface radiation properties of uranium dioxide when in contact with various reactor media. The present study aims to extend their work to include thorium dioxide. Thorium dioxide has renewed interest as a potential reactor fuel, particularly, in view of recent concern about nuclear proliferation.

To use the well known Fresnel relations to calculate surface radiation properties, the values of the complex refractive index ($\hat{n} = n - ik$) of a substance must be provided. The real part of the index, n, is generally called as the index of refraction and the imaginary part, k, as the extinction coefficient. Since the optical constants of ThO_2 are only known at a few selected wavelengths, their values, as one of major purposes of the present study, will be made available over a wide range of the wavelength spectrum. The method to be employed to calculate these optical constants is Kramers-Kronig (K-K) theory, which is a powerful but relatively unknown to heat transfer engineers. A brief review of the theory seems to be in order.

The theory of Kramers-Kronig analysis of reflectance spectra measured with normal incidence on the plane sample was originally described by Robinson,[6] in 1952. Then, in 1967, Berreman[7] extended the applicability of the K-K analysis by presenting an algorithm for computing the phase shifts and n, k from a reflectance spectrum obtained from a radiant flux. The flux was linearly polarized either parallel or perpendicular to the plane of incidence and was specularly reflected at an oblique angle.

In a later work, Didrikil[8] developed a method of K-K analysis for determining the optical constants from the reflectance spectra at an oblique angle of incidence with complete allowance for the degree of polarization, especially zero polarization. For any non-conductor, increasing the angle of incidence continuously increases the component of spectral reflectance. With nonpolarized light a considerable increase in the reflectance takes place for angles of incidence greater than the Brewster angle. In principle, increasing the incidence angle makes it possible to improve the accuracy of measurement of the reflectance in the case where the reflectance at normal incidence is low.

K-K analysis has the advantage of eliminating the need for a polarizer, and increasing the intensity of the reflected light. K-K analysis can be used for any wavelength range, and is suitable to any non-magnetic material. Thus, it simplifies the experimental equipment required and furnishes a better design for the reflection experiment.

This study will discuss two methods that K-K theory can be applied to determine the optical constants from spectral measurement: one from reflection spectra and the other from transmission spectra. After both methods are tested by the classical Lorentz dispersion model, the optical constants of ThO_2 will be determined, followed by evaluating the radiation properties of three types of interfaces:

a. ThO_2 in contact with sodium.

b. ThO_2 in contact with steel.

c. ThO_2 in contact with water vapor.

For each interface, the spectral hemispherical reflectivity will be determined for all wavelengths of interest and the total hemispherical reflectivity from a black body source over a wide temperature range (1200 - 6000°K).

II. ELECTROMAGNETIC THEORY

To begin with, a brief review of reflection laws, primarily Fresnel's relation, from the electromagnetic theory will be made. They will be employed to calculate radiation properties in latter sections.

Fresnel's equations were derived by Fresnel in 1823. On the basis of the elastic theory of light, they give the ratios of the amplitudes of the incident, reflected, and transmitted waves.

Consider two semi-infinite media in direct contact as shown in Fig. 1. They can be either metals or dielectrics, with complex refractive indices $\hat{n}_{1\lambda}$ and $\hat{n}_{2\lambda}$ respectively. The interface between two media is assumed to be specular and optical smooth. The complex index of refraction is shown by $\hat{n}_{\lambda} = n_{\lambda} - ik_{\lambda}$. The subscript λ denotes that $\hat{n}_{\lambda}$, n_{λ} and k_{λ} are, in general, a function of radiation wavelength. According to Fresnel equations, the monochromatic directional reflectance of radiation from medium 1 back to the same medium is

$$\rho_{\lambda\parallel}(\theta) = \tfrac{1}{2}\left(\rho_{\lambda\parallel s}(\theta) + \rho_{\lambda\parallel p}(\theta)\right] \tag{II.1}$$

where

$$\rho_{\lambda\parallel s}(\theta r) = \left| \frac{\hat{n}_{1\lambda}\cos\theta_i - \hat{n}_{2\lambda}\cos\theta_t}{\hat{n}_{1\lambda}\cos\theta_i + \hat{n}_{2\lambda}\cos\theta_t} \right|^2 \tag{II.2}$$

$$\rho_{\lambda\parallel p}(\theta_r) = \left| \frac{\hat{n}_{2\lambda}\cos\theta_i - \hat{n}_{1\lambda}\cos\theta_t}{\hat{n}_{2\lambda}\cos\theta_i + \hat{n}_{1\lambda}\cos\theta_t} \right|^2 \tag{II.3}$$

and $\theta_r = \theta_i$. θ_t can be calculated from Snell's law

$$\hat{n}_{2\lambda}\sin\theta_t = \hat{n}_{1\lambda}\sin\theta_i \tag{II.4}$$

In Eq. (II.1), a circularly polarized light has been assumed, i.e. polarization of the light is assumed to be zero. In case the optical constants are known for all the wavelengths, the spectral directional reflectance over all wavelengths can be found. Then, the monochromatic hemispherical reflectance $\rho_{\lambda 11}$ can be determined by integration over the hemisphere,

$$\rho_{\lambda 11} = 2 \int_0^{\frac{\pi}{2}} \rho_{\lambda 11}(\theta) \sin\theta\cos\theta \, d\theta \qquad \text{(II.5)}$$

and the total hemispherical reflectance can be calculated by integrating over the wavelength,

$$\rho_{11}(T_s) = \frac{\int_0^{\infty} \rho_{\lambda 11} \, H_\lambda(T_s) \, d\lambda}{\int_0^{\infty} H_\lambda(T_s) \, d\lambda} \qquad \text{(II.6)}$$

In Eq. (II.6) H_λ is the incident radiation from a source at temperature T_s. Although the monochromatic reflectance ρ_λ is purely a function of the optical properties, the total reflectance ρ is not, as it depends also on the source temperature T_s. In the absence of a better radiating source, we take it as a black body source at $T_s = T_1$. Thus, the Planck's function serves as a weighting factor. Since it shifts to lower wavelengths as temperature T_s increases, ρ_λ's at lower wavelengths are weighted more than those at higher wavelengths. Generally speaking, the temperature T_s has a significant effect on the reflectance. Care should be taken not to use the temperature of medium 2 on the other side of the interface. Strictly speaking, the optical constants are temperature dependent. However, due to the lack of data at elevated temperature, such temperature dependence could not be accounted for at the present time.

The monochromatic directional transmittance from medium 1 to 2 is given by

$$t_{\lambda 12}(\theta) = 1 - \rho_{\lambda 11}(\theta) \qquad \text{(II.7)}$$

which is the same as the monochromatic directional absorptance of an incident radiation from medium 1 to medium 2.

$$\alpha_{\lambda 12}(\theta) = t_{\lambda 12}(\theta) \qquad \text{(II.8)}$$

In accordance with Kirchnoff's law, the directional monochromatic emittance from medium 2 to 1 is

$$\varepsilon_{\lambda 21}(\theta) = \alpha_{\lambda 12}(\theta) \qquad \text{(II.9)}$$

if $T_1 = T_2$. Therefore, under the condition of a black body source and the condition that $T_2 = T_1$, the total hemispherical properties are inter-related by

$$\rho_{11} = 1 - \alpha_{12} = 1 - \varepsilon_{21} = 1 - t_{12} \qquad \text{(II.10)}$$

Furthermore , the theory can be simplified under these two special cases. They are cited below.

First, if the medium 1 is a dielectric medium such as air or any other gases or vapors, then $k_1 \approx 0$, $n_1 \approx 1$, and $\hat{n}_1 \approx 1$. Upon the substitution of $\hat{n}_1 \approx 1$ into Eq. (II.2) and (II.3) yields expressions quoted by most textbooks.[9-10] This is of particular interest to engineers because the measurements of all the surface properties are conducted by placing the specimen in air, vacuum, or some gaseous media.

The other one is the normal reflectance. When the incident radiation is normal to the interface,

$\theta_i = \theta_r = \theta_t = 0$

Then, from Eqs. (II.1) to (II.4),

$$\rho_{\lambda 11n} = \rho_{\lambda 11p} = \rho_{\lambda 11s} = \left| \frac{\hat{n}_{2\lambda} - \hat{n}_{1\lambda}}{\hat{n}_{2\lambda} + \tilde{n}_{1\lambda}} \right|^2 \qquad \text{(II.11)}$$

which is indeed simple and useful.

In summary, the electromagnetic theory provides a prediction of the monochromatic specular reflectance, from which the spectral specular transmittance and emittance can be inferred, if necessary. Then, spectral and total hemispherical properties can be evaluated.

III. KRAMERS-KRONIG THEORY FOR THE DETERMINATION OF OPTICAL CONSTANTS

In accordance with K-K theory, there are two methods to extract the values of the fundamental spectroscopic parameters, namely, the optical constants n and k, from spectroscopic measurements. The first method is based on a measured reflection spectrum and the second one based on a measured transmission spectrum. The latter is applicable to gaseous media or semi-transparent solids such as ThO_2 or other dielectric materials while the former to solids only, but irrespectively whether the solid is semi-transparent or not, i.e. applicable to dielectrics as well as metals. Even though the second method will not be used in the present study, both methods for the sake of completeness will be described in detail and tested using the classical Lorentz oscillator model. Then, the first method will be employed to calculate the optical constants of ThO_2.

III.1 Optical Constants from Reflection Measurement

III.1.1 Working Formula

According to Fresnel relations, the optical constants n and k can be determined from the spectrum of a perpendicular component R_s by means of the following equations:[8]

$$n = \left\{ \frac{(Q^2-P^2+\sin^2\theta) - \left[(Q^2-P^2+\sin^2\theta)^2 + 4Q^2P^2\right]^{\frac{1}{2}}}{2} \right\}^{\frac{1}{2}} \qquad \text{(III.1)}$$

$$k = PQ/n \qquad \text{(III.2)}$$

where

$$P = \frac{2\sqrt{R_s}\,\sin\phi\cos\theta}{1 + R_s - 2\sqrt{R_s}\,\cos\phi} \qquad \text{(III.3)}$$

$$Q = \frac{(1 - R_s)\cos\theta}{1 + R_s - 2\sqrt{R_s}\,\cos\phi} \qquad \text{(III.4)}$$

and θ is the angle of incidence. Alternatively, P and Q can be expressed in terms of θ, n and k as follows

$$P = nk/Q \qquad \text{(III.5)}$$

$$Q = \left\{\frac{(n^2-k^2-\sin^2\theta) + \left[(n^2-k^2-\sin^2\theta)^2 + 4n^2k^2\right]^{\frac{1}{2}}}{2}\right\}^{\frac{1}{2}} \qquad \text{(III.6)}$$

In the above equations, the phase angle ϕ can be determined from the K-K relationship[11-13]

$$\phi(a) = -\frac{2a}{\pi}\int_0^\infty \frac{\ln\left|\sqrt{R_s(\omega)}\right|}{\omega^2 - a^2}\,d\omega \qquad \text{(III.7)}$$

where ω is an angular frequency, a is the resonance frequency. It relates the phase angle ϕ to the perpendicular component of the specular reflectance R_s, and was obtained from a K-K analysis of an absolute, specular reflectance spectrum of a material. A brief derivation of the phase-shift dispersion relation is given in Appendix B.

The integral relation Eq. (III.7) shows that if the perpendicularly polarized reflectivity R_s is measured over the whole frequency spectrum, the phase angle and the indices n and k can be calculated for any arbitrary frequency at a given incident angle. Performing integration by parts, Eq. (III.7) becomes

$$\phi(a) = \pi^{-1} \int_0^\infty \mathrm{In}\left|\frac{\omega-a}{\omega+a}\right| \frac{d \ \mathrm{In} \ R_s^{\frac{1}{2}}(\omega)}{d\,\omega} d\,\omega \qquad \text{(III.8)}$$

Based on the assumption that the slope of R_s be zero at $\omega=0$ and $\omega=\infty$, we can rewrite Eq. (III.8) into a more convenient form (see Appendix C) as,

$$\phi(a) \doteq \pi^{-1} \sum_{k-2}^{n-1} p_k \left\{(a-\omega_k)\mathrm{In}\left|a-\omega_k\right| + (a+\omega_k)\mathrm{In}\left|a+\omega_k\right|\right\} \qquad \text{(III.9)}$$

where

$$p_k = u_{k+1} - u_k$$

and

$$u_k = \frac{\mathrm{In} \ R_s^{\frac{1}{2}}(\omega_k) - \mathrm{In} \ R_s^{\frac{1}{2}}(\omega_{k-1})}{\omega_k - \omega_{k-1}}$$

The above equation can be easily programmed for numerical computation, a copy of FORTRAN program is given in Appendix E.

By examining Eq. (III.8), we find the values of $R_s(\omega)$ in the spectral regions where $\omega \gg a$ or $\omega \ll a$, do not contribute to the value of $\phi(a)$, because then the weighting function $\mathrm{In}\left\{\left|\omega-a\right| / (\omega+a)\right\}$ approaches zero. Thus, we can neglect the variations of the reflectance spectrum, even if the variations are reasonably large, in those region. Consequently, we can assume the reflectance flatten out on both ends of spectrum. Moreover, in view that the spectral region in which the reflectance is constant do not contribute to the value of $\phi(a)$, only a finite spectral region of the reflectance spectrum needed to be measured, which reduces experimental efforts considerably.

The reflectance measured in the experiment is not R_s, but is R_o

given by

$$R_o = \frac{1}{2}\left[R_s(1+\alpha) + R_p(1-\alpha)\right] \tag{III.10}$$

where α is the degree of polarization

$$\alpha = \frac{I_s - I_p}{I_s + I_p}$$

I_s and I_p are the reflected intensities of light in the planes perpendicular and parallel to the plane of incidence respectively. We can rewrite Eq. (III.10) in the form

$$R_s = \frac{2R_o}{(1+\alpha) + (R_p/R_s)(1-\alpha)} \tag{III.10.a}$$

Because we are interested in using a nonpolarized light, $\alpha=0$. The ratio R_p/R_s in turn is defined in the terms of P, Q and θ as

$$\frac{R_p}{R_s} = \frac{(Q-\sin\theta\tan\theta)^2 + P^2}{(Q+\sin\theta\tan\theta)^2 + P^2} \tag{III.11}$$

Also,

$$R_s = \frac{(Q-\cos\theta)^2 + P^2}{(Q+\cos\theta)^2 + P^2} \tag{III.11.a}$$

III.1.2 Direct Method

If we can determine the ratio R_p/R_s and knowing the value of polarization α through the experiment, then it is possible to calculate the R_s spectrum directly from the measured reflectance R_o using Eq. (III.10.a). The optical constants can then be calculated from Eqs. (III.1) and (III.2) with P and Q from Eqs. (III.3) and (III.4). However, it is not simple to determine the ratio R_p/R_s because R_s is unknown.

In order to determine the ratio R_p/R_s, experimental setup is somewhat complicated and expensive as the source light has to be polarized. Therefore, this method is avoided whenever possible. Instead the following method is more favorable.

III.1.3 Iterative Method

For the determination of the optical constants from the measured R_o spectrum, we use the method of successive approximations suggested by Ref. 8. We can substitute R_o in place of R_s in Eqs. (III.3), (III.4) and (III.7). The values of $\phi(a)$ obtained are used to calculate the zeroth approximation of P and Q from Eqs. (III.3) and (III.4), and R_p/R_s from Eq. (III.11). Based on the R_p/R_s value, the first approximation of R_s^* is obtained from Eq. (III.10.a) which is then used to redetermine ϕ, P, Q, R_p/R_s and the next approximation of R_s^* until convergence is reached. The final set of R_s^* is the desired R_s. Therefore, this process of successive approximations makes it possible to obtain the R_s spectrum from R_o spectrum with the required degree of accuracy and certain imposed conditions to be discussed later.

In certain wavelength range, sustained oscillations of the values of R_s^* may be produced, so the suggestions made by Ref. 8 can be followed. Since the difference between $R_s^*-R_s$ in the ith and (i-1)th iteration have different signs, we introduce the additional condition

$$R_s^*(i) = \tfrac{1}{2}[R_s^*(i) + R_s^*(i-1)] \qquad \text{(III.12)}$$

to expedite the convergence. The above equation means that, in the process of iteration, instead of using the newly obtained R_s^* value from (i-1)th iteration for ith iteration, a weighted average with the previous value should be used. Equation (III.12) is used only for the calculation of those R_s^* which the corresponding R_o exceed a certain value B. The number of iterations for convergence depends on the choice of B, and increases with an increase in the incidence angle.

For the reflectance with a high maximum of R_o, R_{max}, and a relatively low edge, the value of B can be taken as $R_{max}/2$. For spectra with low R_{max} and a high long wave edge, the lower limit of B can be taken as the value of C, where $C = (R_{ok}+R_{max})/2$. R_{ok} is the value of the reflectivity of long wave edge at a sufficient distance from the reflection band. In the intermediate case, B has a value lying between $R_{max}/2$ and C. In practice, it is better not to use Eq. (III.12) in the first iteration. Instead it is applied to all points of the spectrum after 4-6 iterations. Or, simply setting B=C in the first 4-6 cycles, then apply Eq. (III.12) to all the points of R_s^* spectrum.[8]

As to the selection of the angle of incidence θ, we use the value of the normal reflectivity at the maximum of the reflectance band, R_n, as a criterion. For high values of R_n, on the order of 0.9, the use of an oblique incidence angle may prove useful, though it is necessary to restrict the angle of θ not to exceed 60°. For R_n less than the order of 0.1, the angle θ may reach 80°. In the intermediate cases, it is convenient to select θ around 70°.

To test the validity of the iterative method for the determination of R_s and therefore the optical constants from Eqs. (III.1) to (III.5) from R_o spectrum, the classical Lorentz oscillator model is used. Details about the oscillator can be found in Appendix A.

Let us take the oscillator equations which best fit the reflectivity data of the material α-IISiC for example. The four correlation parameters in the equations for this material have been found as[14]

$\rho = 0.263$

$\gamma = 0.006$

$a = 12.60$

$\varepsilon_0 = 6.7$

With these parameters, n and k of α-IISic can be calculated from Eqs. (A.17) to (A.21) in Appendix A and the results are listed in the last two columns of Table 1. Also can be calculated are P and Q from Eqs. (III.5) and (III.6), respectively. Finally by choosing a non-polarized light, $\alpha=0$, and an incidence angle of $\theta=60^\circ$ or $\theta=70^\circ$, R_0 and R_s reflection spectra can be calculated through the use of Eqs. (III.11) and (III.11.a). They are displayed in Fig. 2 and listed in Table 1 as well.

Using the R_0 spectrum and the iterative method as just described, the values of R_s^*, n^* and k^* at the end of the iteration are shown in Table 2 and Figs. 3 and 4. By comparing those in Table 2 with R_s, n and k values in Table 1 or by examining Figs. 3 and 4, we see that, for the case of $\theta=70^\circ$, they are in good agreement everywhere except near the peak region between 11 and 13 . The sustained oscillations of R_s^* can not be avoided even if the additional condition, Eq. (III.12), is used. One possible reason is that the incidence angle is too high. If we check the reflectance spectra, there are many reflectance exceed the value of 0.95. In this instance, the incidence angle should be restricted to 60° or less. As we examine the case with $\theta=60^\circ$, we find the results in figs. 3

and 4 not only converge everywhere but also in good agreement through the whole spectrum. Thus the iterative K-K analysis can be successfully applied in determining the optical constants directly from the experimental reflection spectra.

As stated in Ref. 8, it should be mentioned in passing that the magnitude of error depends on the ratio of R_p/R_s. If both polarization α and R_p/R_s are zero, the magnitude of error reaches a maximum. When a nonpolarized light is used in an experiment, α is equal to zero, then the ratio R_p/R_s becomes critical to the accuracy of the iterative method using the K-K analysis.

III.2 Optical Constants from Transmission Measurement

In the thin-film theory, the absorption coefficient, K_a, which describes the fractional decrease in intensity I with distance s, is defined as

$$K_{a\lambda} = -\frac{1}{I}\frac{dI}{ds} \qquad \text{(III.13)}$$

Therefore,

$$K_{a\lambda} = \frac{\ln(I_o/I)}{s} = \frac{2.303 \times \text{O.D.}}{s} \qquad \text{(III.14)}$$

where: I_o - is the intensity of the light beam before shining onto the sample.

s - sample thickness.

O.D. - optical density.

From the above, $K_{a\lambda}$ can be evaluated from transmission or absorption spectra which describe the optical density as a function of λ. Then one of the optical constants, namely, the extinction coefficient k, can be evaluated from $K_{a\lambda}$ by the relation

$$k = K_{a\lambda}\lambda/4\pi \qquad \text{(III.15)}$$

To evaluate the other optical constant, the K-K dispersion relations are introduced. They are integral relations between the real and imaginary parts of a function $f(\omega)$ which is frequency dependent, and analytic in the upper half of the complex frequency plane. For a given frequency a, these relations can be written:[15]

$$\operatorname{Re} f(a) = \frac{2}{\pi}\,\text{p.v.}\int_0^\infty \frac{\omega \operatorname{Im} f(\omega)}{\omega^2 - a^2}\,d\omega \qquad \text{(III.16)}$$

$$\operatorname{Im} f(a) = -\frac{2}{\pi}\,\text{p.v.}\int_0^\infty \frac{\operatorname{Re} f(\omega)}{\omega^2 - a^2}\,d\omega \qquad \text{(III.17)}$$

where: p.v. signifies principle value of the integral for $\omega = a$.

These relations are valid for any physical quantity which expresses a linear relation between the response of system and the incident excitation, under the condition that the response of a system could never preceed the incident excitation. These relations are useful if the complex function of $f(\omega)$ is replaced by the complex index, $\hat{n}(\omega) = n(\omega) - iK(\omega)$. We have,

$$n(a) = \frac{2}{\pi}\,\text{p.v.}\int_0^\infty \frac{\omega k(\omega)}{\omega^2 - a^2}\,d\omega \qquad \text{(III.18)}$$

$$k(a) = -\frac{2}{\pi}\,\text{p.v.}\int_0^\infty \frac{n(\omega)}{\omega^2 - a^2}\,d\omega \qquad \text{(III.19)}$$

If either $n(\omega)$ or $k(\omega)$ function is known, the other function can be determined directly through one of the integrals. Consequently, we don't really have to measure the reflectances for certain crystals if the transmission spectra are known, because from the transmission spectra the absorption coefficient $K_{a\lambda}$ can be calculated from Eq. (III.14) as a function of frequency. Therefore, the extinction coefficients can be calculated from Eq. (III.15), and $n(\omega)$ from Eq. (III.18).

Similar to Eq. (III.7), Eqs. (III.16) and (III.17) can be expressed in the following conveniently numerical forms,[15]

$$n(a) - n(\infty) = \frac{1}{\pi}\sum_{k=2}^{n-1} q_k \left[(a-\omega_k)\ln\left|a-\omega_k\right| - (a+\omega_k)\ln(a+\omega_k)\right] \quad \text{(III.20)}$$

$$k(a) = -\frac{1}{\pi}\sum_{k=2}^{n-1} p_k \left[(a-\omega_k)\ln\left|a-\omega_k\right| + (a+\omega_k)\ln(a+\omega_k)\right] \quad \text{(III.21)}$$

where: ω_k - the frequency of a pole of a partial fraction.
q_k - the variation of the slope of $k(\omega)$ at these points.
p_k - the variation of the slope of $n(\omega)$ at these points. (see Appendix C)

It should be mentioned that any error in the determination of a measured function, even if it occurs only at a single frequency, will affect the whole assembly of the calculated values of the other function. In particular, the inherent assumption of zero slope at both integration limits in Eqs. (III.20) and (III.21) should be carefully observed by setting, for example, $k_1=k_2$ and $k_{n-1}=k_n$ in Eq. (III.20).

Noting that in the calculation of surface radiation properties, the refractive index n is dominant. Therefore, it is better off not to assume n to be constant. Instead a more realistic refractive index function, $n(\lambda)$, which varies with frequency should be used wherever possible. Thus Eq. (III.20) is of particular importance since it can be used to generate n values from k values.

To test Eq. (III.20), the values of the extinction coefficient k of Lorentz model listed in Table 1 are used in the equation to see if the reproduced index of refraction n^* agrees with the original n listed in Table 1. The results are compared in Table 3 and displayed in Fig. 5. It shows that the agreement is remarkably good.

IV. COMPUTATION & RESULT

Being sucessfully verified in the previous section, the K-K theory can now be employed to calculate the optical constants of thorium dioxide. It will then be followed by the calculation of surface radiation properties of thorium dioxide when it is in direct contact with sodium, steel or a gas.

IV.1 Optical Constants of Thorium Dioxide

Theorectically speaking, the optical constants of ThO_2 can be calculated by the equations from the Lorentz theory of dielectric media. However, in practical applications, we find the equations tend to fail for non-monatomic solids as it is difficult to fit data through the equations even if the criteria described in Appendix A.1 are followed. The calculated k values are found to deviate greatly from the experimental absorption spectrum at different temperatures.

a. Extinction Coefficient k:

According to Ref. 16, Bates reported the absorption spectra of a single crystal ThO_2 at room temperature from the wavelength range 2 to 13μ with 0.048 cm sample thickness. Also, he measured sample at high temperature with different annealed gases from 0.2 to 5μ. The extinction coefficient k, therefore, can be determined from the optical density by Eq. (III.14). The absorption spectra are reproduced in three figures in Appendix D.

b. Index of Refraction n:

Once the extinction coefficient is known, the K-K dispersion theory is applied to find the real part of the complex refractive index, namely, the index of refraction n. The difference between $n(\infty)$ and $n(\omega)$ is first calculated from Eq. (III.20). In order to determine the values of n(ω), we have to determine the n(∞) next. As far as n(∞) is concerned, it is the square root of ε_o (see Eq. (A.13) in Appendix A). Because the value of ε_o for ThO_2 is not available, we have to interpolate the value from other means. Ellis & Lindstrom[17] reported the index of refraction as following: 5893 Å, n=2.105±0.005; 5641 Å, n=2.110±0.005; 4358 Å, n=2.135±0.005. Since the values of the integral term on the right hand side of Eq. (III.20) can be calculated at any of those three wavelengths, n(∞) can be evaluated from Eq. (III.20). A value of n(∞) =2.072 seems to fit well at all three wavelengths. With this n(∞) value, n(ω) at all wavelengths can be readily calculated as shown in Table 4. The results in the table show that the index of refraction varies only slightly with wavelengths.

IV.2 Optical Constants of Sodium & Steel

The Drude model for metals is obtained directly from the Lorentz model simply by setting a equal to zero in Eq. (A.13) and (A.14)

$$n^2 - k^2 = \varepsilon_o - \frac{4\pi Ne^2}{m} \frac{1}{(\omega^2 + \gamma^2)}$$

$$2nk = \frac{4\pi Ne^2}{m} \frac{\gamma}{(\omega^2 + \gamma^2)}$$

a. Sodium

According to Chan and Tseng[5], $(4\pi Ne^2/m)^{0.5}$ is 8.9×10^{15} sec^{-1}, and the optimum value of γ appears to be 5.142×10^{13} sec^{-1}. They computed the optical constants using the above equations and the results are drafted in Fig. 6 and Table 5 for convenient. The calculated value of the optical constant at λ=0.2μ is replaced by the same value as that at λ=0.25μ

due to obvious error discussed in Ref. 5.

b. Steel

Again in Chan and Tseng's work, the optimal values $(4\pi Ne^2/m)^{0.5}$ and γ of steel are found to be 2.005×10^{16} $\sec^{-1}$ and 8.26×10^{15} $\sec^{-1}$, respectively. The resulting optical constants are shown in Fig. 7 & Table 6.

IV.3 Spectral Hemispherical Reflectance

Knowing the optical constants of the two contacting materials, it is possible to calculate the spectral hemispherical properties from Eqs. (II.1) to (II.5). The 20-point Gaussian Quadrature is used to integrate Eq. (II.5) to yield the spectral hemispherical reflectance. A sample FORTRAN program is presented in Appendix F.

IV.4 Total Hemispherical Properties

The total hemispherical properties can be calculated from the spectral hemispherical properties by Eqs. (II.6) to (II.10). The trapezoidal method with 44 integration points between 0.2 and 10 is used to evaluate the spectral integral in the equations with a black source temperature ranging from 1200°K to 6000°K.

IV.5 Summary

In general, the radiation properties from the medium 1 side are different from the medium 2 side. It is necessary to indicate from which medium the radiation originates and to which medium it ends up.

In this study we always choose to originate from medium 1 to 2 (subscript "12"). By Kirchhoff's law the spectral absorptance $\alpha_{\lambda 12}$ equals the spectral hemispherical emittance from medium 2, $\varepsilon_{\lambda 21}$. Since we take the radiation source as a black body at the same temperature as both media in contact, the total hemispherical absorption α_{12} is equal to the total hemispherical emittance ε_{21}.

IV.5.1 ThO_2-Sodium Interface (medium 1-ThO_2, medium 2-Sodium)

In reactor safety analysis, it often concerns with the intereaction between a molten fuel and a reactor coolant. When a molten ThO_2 drops into a liquid sodium, direct contact occurs and the radiation properties at the ThO_2-sodium interface will be needed for calculating radiative cooling from ThO_2. The calculated spectral hemispherical properties of this interface are given in Table 7 and Fig. 9 while the total hemispherical properties of the interface are given in Table 8 and Fig. 10.

IV.5.2 ThO_2-Steel Interface (medium 1-ThO_2, medium 2-Steel)

When a molten ThO_2 is in direct ocntact with a reactor material such as stainless steel, the properties of ThO_2-Steel interface would be of interest. Since the optical constants available are for the steel (99Fe + 1C) but not for the stainless steel, we can only calculate the properties of ThO_2-Steel (99Fe + 1C) interface. The spectral hemispherical properties of the contact interface are given in Table 9 and Fig. 11 while the total hemispherical properties of the interface are given in Table 10 and Fig. 12.

IV.5.3 Gas-ThO_2 Interface (medium 1-Gas, medium 2-ThO_2)

This interface exists when a vapor film (or any gas film) separates ThO_2 from sodium or water. The spectral hemispherical properties of such an interface are given in Table 11 and Fig. 13 while the total hemispherical properties of the interface given in Table 12 and Fig. 14.

V. COMPARISON & DISCUSSION

The optical constant of thorium dioxide and the radiation properties of three types of interfaces, namely, ThO_2-Sodium, ThO_2-Steel and Gas-ThO_2, have been calculated in the last section. A number of issues concerning those properties will be discussed here, and a comparison of the results will be made with experimental data or other analytical results that are currently available.

V.1 ThO_2-Sodium Radiation Properties

As for the total hemispherical reflectance of ThO_2-Sodium, our calculation (see Fig. 10) shows that it lies in the range of 0.9766 to 0.9903 as the temperature increases from 1200°K to 6000°K. From Table 7, it is clear that the spectral hemispherical values may not be accurate at extremely short wavelengths, say $\lambda \leq 0.2\mu$ due to the inherent error in the optical constants of sodium (see Table 5). Fortunately, the possible error has practically no effect on total radiation property calculations because less than 0.5% of black body radiation energy lies in the region $\lambda \leq 0.2\mu$ even if the black body is at a temperature as high as 6000°K. No results are available for comparison, nor any experimental data are available since a direct measurement of, say, reflection from an interface is possible only when one side of the interface is vacuum or a gas.

V.2 ThO_2-Steel Radiation Properties

From the analysis, we report the values of spectral and total hemispherical reflectance of ThO_2-Steel interface in Table 9 & 10, respectively. Because the spectral hemispherical reflectance in the long wavelength region weights more in Eq. (II.6) as temperature increases, the total hemispherical reflectance increases with temperature. Again no comparison can be made in this case.

V.3 Gas-ThO_2 Radiation Properties

1) Spectral Hemispherical Properties

We report that the value of the reflectance is essentially constant, 0.174. Since the index of refraction is dominant in determining the radiation properties and the indices of refraction of both the interfaces change very little ($n_1 = 1$, $n_2 = 2.11$), a constant value is therefore expected. Some experimental values of normal spectral emissivity of thorium dioxide (thoria) were reported in connection with early works on thoria cathodes emission about thirty years ago. They vary over a wide range such as 0.35,[22] 0.2 to 0.7[23] at $\mu = 0.65$ while 0.35 was also assumed by Ref. 24 to determine thoria surface temperature from pyrometer measurements. Those values, nevertheless, can not be used for comparison with the present analytical calculations because they are the spectral emissivity from a thin coat of thoria on molybdenum[22], tungsten[23] or tantalm.[24] Since the coating thickness is only 0.025 to 0.038 mm[22], 0.05 mm[23] or 0.1 mm[24] and the extinction coefficient of thoria is about 26 cm^{-1}, the thoria coating is obviously in the optically thin region that the radiation from the base metal penetrates through the coating. Therefore, the reported spectral emissivities do not represent that of a bulk thoria.

2) Total Hemispherical Properties

We integrate the spectral hemispherical reflectance of Gas-ThO_2 interface to obtain the total hemispherical reflectance from 1200°K to 6000°K, and find 0.1741 at 1200°K; 0.1750 at 6000°K (see Fig. 14). Again in connection with the investigations on thoria-coated cathodes, total normal emissivity was reported as 0.5[24] with a thoria thickness of 0.5 mm at 1900°K. Reference 25 claimed between 0.2 to 0.6 in the temperature range of 250 to 800°C for a sintered thoria with an unspecified thickness. Though comparison with the present calculation, which is valid for a pure bulk thoria with an optically smooth surface, may not meaningful for the same reason stated above, it may be appropriate to point out that the total normal reflectivity calculated from Eq. (II.11) is about 0.13 which would lead to a total normal emissivity of 0.87, higher than either reported values. Also should be pointed out is the inherent limitation imposed on the present calculation, namely, the optical constants used were derived from low temperature data (mainly the room temperature) as no higher temperature data are available. Thus the temperature dependence of optical constants can not be accounted for in the present investigation.

VI. CONCLUSION

The present study continues Chan and Tseng's work[5] in providing the surface radiation properties of reactor materials that are useful in the safety analysis of nuclear reactors. Two methods of using K-K theory to calculate the optical constants from measured reflection and transmission spectra have been put into practical use. In particular, the optical constants of thorium dioxide have been calculated and presented here. Also presented are the spectral and total hemispherical properties of thorium dioxide in contacting with sodium steel or a gas. The spectral hemispherical properties are presented over a wide spectral range while the total hemispherical properties over a temperature range of 1200°K to 6000°K.

Table 1

Reflectance Spectra of the Classical Dispersion for $\alpha = 0$

Wavelength λ (μ)	Reflectance in Perpendicular Direction R_s		Experimental Reflectance R_σ		Index of Refraction n	Extinction Coefficient k
	$\theta = 60^\circ$	$\theta = 70^\circ$	$\theta = 60^\circ$	$\theta = 70^\circ$		
2.0	0.4326	0.5625	0.2282	0.2816	2.572	0.0
3.0	0.4290	0.5592	0.2259	0.2801	2.550	0.0
4.0	0.4233	0.5541	0.2222	0.2777	2.516	0.0
5.0	0.4148	0.5463	0.2167	0.2742	2.466	0.00035
6.0	0.4019	0.5345	0.2087	0.2689	2.394	0.00073
7.0	0.3815	0.5155	0.1963	0.2607	2.286	0.00155
8.0	0.3460	0.4816	0.1757	0.2465	2.114	0.00337
9.0	0.2705	0.4054	0.1353	0.2156	1.805	0.00834
10.0	0.0082	0.0280	0.0049	0.0209	1.038	0.03485
10.5	0.9472	0.9650	0.9120	0.9377	0.068	0.90216
11.0	0.9781	0.9852	0.9556	0.9620	0.059	1.972
11.5	0.9847	0.9896	0.9658	0.9658	0.078	2.865
12.0	0.9856	0.9901	0.9659	0.9612	0.196	5.046
12.2	0.9842	0.9892	0.9623	0.9552	0.350	6.526
12.4	0.9800	0.9863	0.9517	0.9404	0.958	9.612
12.6	0.9412	0.9594	0.8631	0.8310	16.70	16.49
12.8	0.8273	0.8784	0.6471	0.6016	10.51	0.9323
13.0	0.7727	0.8382	0.5631	0.5242	7.801	0.3325
14.0	0.6600	0.7524	0.4214	0.4106	4.907	0.0503
15.0	0.6157	0.7174	0.3754	0.3777	4.234	0.0227

Table 2

Optical Constants by K-K Theory Using Iterative Method

Wavelength λ (μ)	R_s^*		n^*		k^*	
	$\theta = 60°$;	$\theta = 70°$	$\theta = 60°$;	$\theta = 70°$	$\theta = 60°$;	$\theta = 70°$
2.0	0.4325	0.5624	2.571	2.571	0.0212	0.0188
3.0	0.4290	0.5592	2.550	2.550	0.0217	0.0183
4.0	0.4233	0.5540	2.516	2.515	0.0254	0.0216
5.0	0.4147	0.5463	2.465	2.466	0.0288	0.0233
6.0	0.4019	0.5344	2.394	2.393	0.0276	0.0204
7.0	0.3815	0.5155	2.285	2.285	0.0389	0.0309
8.0	0.3460	0.4816	2.113	2.113	0.0384	0.0297
9.0	0.2704	0.4053	1.804	1.804	0.0287	0.0204
10.0	0.0080	0.0272	1.012	1.017	0.0457	0.0430
10.5	0.9469	0.9648	0.068	0.068	0.8680	0.8794
11.0	0.9779	*	0.056	*	1.898	*
11.5	0.9845	0.9896	0.086	0.087	3.176	3.156
12.0	0.9854	*	0.169	*	4.649	*
12.5	0.9734	*	1.741	*	11.158	*
12.6	0.9411	*	8.597	*	14.438	*
12.7	0.8707	0.9078	12.195	7.269	5.250	7.031
12.8	0.8272	0.8771	9.860	8.234	2.659	4.256
13.0	0.7726	0.8372	7.569	7.120	1.342	2.018
13.5	0.6998	0.7826	5.602	5.509	0.660	0.8934
14.0	0.6599	0.7515	4.858	4.808	0.4713	0.6368
15.0	0.6155	0.7166	4.189	4.171	0.4044	0.4394

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* divergence

Table 3

Index of Refraction from the Values of Extinction Coefficient by Integral K-K Dispersion Relations

Wavelength λ (μ)	Index of Refraction from K-K Analysis n^*	Index of Refraction n	Extinction Coefficient k
5.0	2.516	2.466	0.00035
6.0	2.441	2.394	0.00073
7.0	2.331	2.286	0.00155
8.0	2.156	2.114	0.00337
9.0	1.842	1.805	0.00834
10.0	1.046	1.038	0.03485
11.0	0.0853	0.059	1.972
12.0	0.1760	0.196	5.046
12.1	0.2216	0.254	5.686
12.2	0.3010	0.350	6.526
12.3	0.4604	0.532	7.713
12.4	0.8756	0.958	9.612
12.5	3.419	2.592	13.412
12.6	12.323	16.70	16.495
12.7	15.590	14.04	2.498
12.8	11.001	10.51	0.9323
12.9	9.086	8.815	0.5115
13.0	7.979	7.801	0.3325
14.0	4.996	5.684	0.0503
15.0	4.307	4.234	0.0227
16.0	3.989	3.924	0.0138

Table 4

Optical Constants of ThO_2

Wavelength λ (μ)	Index of Refraction n	Extinction Coefficient k
0.20	2.118	0.0003053
0.25	2.117	0.0001717
0.30	2.116	0.0001694
0.35	2.116	0.0001376
0.40	2.115	0.0001374
0.45	2.114	0.0001168
0.50	2.114	0.0001202
0.55	2.114	0.0001322
0.60	2.113	0.0001488
0.65	2.113	0.0001637
0.70	2.113	0.0001736
0.75	2.112	0.0001717
0.80	2.112	0.0001526
0.85	2.112	0.0001297
0.90	2.112	0.0001030
0.95	2.111	0.0000906
1.00	2.111	0.0000763
1.05	2.111	0.0000641
1.10	2.111	0.0000545
1.15	2.111	0.0000482
1.20	2.111	0.0000458
1.25	2.111	0.0000452

Table 4 (Cont'd)

Wavelength λ (μ)	Index of Refraction n	Extinction Coefficient k
1.30	2.111	0.0000446
1.35	2.111	0.0000436
1.40	2.111	0.0000427
1.45	2.110	0.0000385
1.50	2.110	0.0000343
2.00	2.108	0.0000191
2.50	2.107	0.0000275
3.00	2.107	0.0000435
3.50	2.106	0.0000372
4.00	2.105	0.0000305
4.50	2.105	0.0000326
5.00	2.104	0.0000471
5.50	2.104	0.0000242
6.00	2.103	0.0000092
6.50	2.103	0.0
7.00	2.102	0.0
7.50	2.102	0.0
8.00	2.101	0.0000519
8.50	2.100	0.00026
9.00	2.099	0.000515
9.50	2.099	0.002624
10.00	2.099	0.003513

Table 5

Optical Constants of Sodium

Wavelength λ (μ)	Index of Refraction n		Extinction Coefficient k	
	Present	References	Present	References
0.20	0.007		0.008	
0.25	0.007	0.025*(18)	0.646	0.585*(18)
0.30	0.008	0.036*(18)	1.020	0.944*(18)
0.35	0.009	0.043*(18)	1.333	1.319*(18)
0.40	0.012	0.047*(18)	1.621	1.545*(18)
0.45	0.014	0.045*(18) 0.058*(19)	1.895	1.866*(18) 1.864*(19)
0.50	0.017	0.036*(18) 0.060*(19)	2.177	2.102*(18) 2.092*(19)
0.55	0.021	0.052*(19) 0.047*(20)	2.420	2.229*(19) 2.238*(20)
0.60	0.024	0.045*(19)	2.676	2.476*(19)
0.65	0.029	0.049*(19)	2.929	2.733*(19)
0.70	0.033		3.180	
0.75	0.038		3.429	
0.80	0.043		3.676	
0.85	0.048		3.922	
0.90	0.054		4.167	
0.95	0.062		4.265	
1.00	0.066		4.656	
1.05	0.070		4.899	
1.10	0.080		5.141	
1.15	0.087		5.384	
1.20	0.094		5.626	
1.25	0.102		5.868	
1.30	0.111		6.110	

Table 5 (Cont'd)

Wavelength λ (μ)	Index of Refraction n		Extinction Coefficient k	
	Present	References	Present	References
1.35	0.119		6.351	
1.40	0.128		6.591	
1.45	0.138		6.833	
1.50	0.147		7.074	
2.00	0.261		9.474	
2.25		0.410 (18)		11.60 (18)
2.50	0.407	0.500 (18)	11.855	12.50 (18)
3.0	0.585	0.610 (18)	14.261	14.70 (18)
3.5	0.795	0.810 (18)	16.655	17.20 (18)
4.0	1.038	1.020 (18)	19.049	19.40 (18)
4.5	1.260		22.355	
4.75		1.71 (18)		22.30 (18)
5.0	1.621		23.843	
5.5	1.961		26.251	
6.0	2.331		28.648	
6.5	2.734		31.056	
7.0	3.169		33.468	
7.2		3.66 (18)		32.9 (18)
7.5	3.636		35.881	
8.0	4.134		38.305	
8.5	4.633		40.731	
9.0	5.223		43.162	
9.5	5.815		45.599	
10.0	6.437		48.041	

Table 6

Optical Constants of Steel (99 Fe + 1 C)

Wavelength λ (μ)	Index of Refraction n		Extinction Coefficient k	
	Present	References	Present	References
0.20	0.806		1.626	
0.25	1.048	1.353*(18)	1.963	1.818*(18)
0.30	1.281	1.397*(18)	2.237	2.008*(18)
0.35	1.501	1.472*(18)	2.466	2.357*(18)
0.40	1.707	1.680*(18)	2.666	2.721*(18)
0.45	1.898	1.895*(18)	2.842	2.927*(18)
0.50	2.078	2.130*(18)	3.001	3.109*(18)
0.55	2.246	2.327*(18)	3.149	3.261*(18)
0.60	2.405	2.490*(18)	3.286	3.337*(18)
0.65	2.555	2.615*(18)	3.414	3.434*(18)
0.70	2.700	2.700(18)	3.537	3.537(18)
0.75	2.834		3.651	
0.80	2.964		3.762	
0,85	3.089		3.868	
0.90	3.210		3.971	
0.95	3.326		4.070	
1.00	3.438		4.167	
1.05	3.547		4.261	
1.10	3.653		4.352	
1.15	3.755		4.441	
1.20	3.855		4.528	
1.25	3.953		4.613	
1.30	4.047		4.696	

Table 6 (Cont'd)

Wavelength λ (μ)	Index of Refraction n		Extinction Coefficient k	
	Present	References	Present	References
1.35	4.140		4.778	
1.40	4.231		4.858	
1.45	4.320		4.937	
1.50	4.456		5.073	
2.00	5.200		5.723	
2.50	5.880		6.356	
3.00	6.494		6.929	
3.50	7.049		7.452	
4.00	7.566		7.943	
4.50	8.049		8.405	
5.00	8.505		8.843	
5.50	8.937		9.260	
6.00	9.350		9.659	
6.50	9.745		10.042	
7.00	10.125		10.410	
7.50	10.491		10.766	
8.00	10.844		11.111	
8.50	11.186		11.446	
9.00	11.518		11.771	
9.50	11.841		12.086	
10.00	12.155		12.395	

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* Interpolated Values.

Table 7

ThO_2-Sodium Interface Spectral Hemispherical Properties (medium 1-ThO_2 ; medium 2-Sodium)

Wavelength λ (μ)	$\alpha_{\lambda 12}$	$\rho_{\lambda 11}$
0.20	0.48338	0.51662
0.25	0.00559	0.99441
0.30	0.00731	0.99269
0.35	0.00816	0.99183
0.40	0.01031	0.98969
0.45	0.01116	0.98884
0.50	0.01237	0.98763
0.55	0.01403	0.98597
0.60	0.01464	0.98536
0.65	0.01613	0.98387
0.70	0.01675	0.98325
0.75	0.01763	0.98237
0.80	0.01827	0.98173
0.85	0.01872	0.98128
0.90	0.01937	0.98063
0.95	0.02149	0.97851
1.00	0.02020	0.97980
1.05	0.01988	0.98012
1.10	0.02112	0.97888
1.15	0.02140	0.97860
1.20	0.02159	0.97841

Table 7 (Cont'd)

Wavelength λ (μ)	$\alpha_{\lambda 12}$	$\rho_{\lambda 11}$
1.25	0.02193	0.97807
1.30	0.02237	0.97763
1.35	0.02253	0.97747
1.40	0.02282	0.97718
1.45	0.02317	0.97683
1.50	0.02330	0.97670
2.00	0.02504	0.97496
2.50	0.02616	0.97384
3.00	0.02683	0.97317
3.50	0.02731	0.97269
4.00	0.02768	0.97232
4.50	0.02488	0.97512
5.00	0.02819	0.97191
5.50	0.02835	0.97165
6.00	0.02847	0.97153
6.50	0.02853	0.97147
7.00	0.02857	0.97143
7.50	0.02861	0.97139
8.00	0.02861	0.97139
8.50	0.02843	0.97157
9.00	0.02859	0.97141
9.50	0.02877	0.97123
10.00	0.02878	0.97122

Table 8

ThO_2-Sodium Interface Total Hemispherical Properties (medium 1-ThO_2 ; medium 2-Sodium)

Temperature (^oK)	α_{12}	ρ_{11}
1200	0.02337	0.97663
1400	0.02239	0.97761
1600	0.02145	0.97855
1800	0.02054	0.97946
2000	0.01967	0.98033
2200	0.01884	0.98116
2400	0.01804	0.98196
2600	0.01729	0.98271
2800	0.01658	0.98342
3000	0.01591	0.98409
3200	0.01527	0.98743
3400	0.01468	0.98532
3600	0.01412	0.98588
3800	0.01360	0.98640
4000	0.01312	0.98688
4200	0.01266	0.98734
4400	0.01223	0.98777
4600	0.01183	0.98817
4800	0.01146	0.98854
5000	0.01111	0.98889
5400	0.01049	0.98951
5800	0.00994	0.99006
6000	0.00970	0.99030

Table 9

ThO_2-Steel Interface Spectral Hemispherical Properties (medium 1-ThO_2 ; medium 2-Steel)

Wavelength λ (μ)	$\alpha_{\lambda 12}$	$\rho_{\lambda 11}$
0.20	0.48194	0.51806
0.25	0.53290	0.46710
0.30	0.56324	0.43676
0.35	0.58165	0.41835
0.40	0.59233	0.40767
0.45	0.59815	0.40185
0.50	0.60107	0.39893
0.55	0.60152	0.39848
0.60	0.60061	0.39939
0.65	0.59880	0.40120
0.70	0.59627	0.40373
0.75	0.59320	0.40680
0.80	0.58981	0.41019
0.85	0.58620	0.41380
0.90	0.58256	0.41744
0.95	0.57867	0.42133
1.00	0.57473	0.42527
1.05	0.57083	0.42917
1.10	0.56698	0.43302
1.15	0.56310	0.43690
1.20	0.55927	0.44073
1.25	0.55551	0.44449

Table 9 (Cont'd)

Wavelength λ (μ)	$\alpha_{\lambda 12}$	$\rho_{\lambda 11}$
1.30	0.55177	0.44823
1.35	0.54806	0.45194
1.40	0.54445	0.45555
1.45	0.54074	0.45926
1.50	0.53419	0.46581
2.00	0.50549	0.49451
2.50	0.47873	0.52127
3.00	0.45646	0.54354
3.50	0.43748	0.56252
4.00	0.42087	0.57913
4.50	0.40637	0.59363
5.00	0.39335	0.60665
5.50	0.38177	0.61823
6.00	0.37117	0.62883
6.50	0.36162	0.63838
7.00	0.35278	0.64722
7.50	0.34472	0.65528
8.00	0.33715	0.66285
8.50	0.33011	0.66989
9.00	0.32355	0.67645
9.50	0.31778	0.68222
10.00	0.31217	0.68783

Table 10

ThO_2-Steel Interface Total Hemispherical Properties (medium 1-ThO_2 ; medium 2-Steel)

Temperature (°K)	α_{12}	ρ_{11}
1200	0.52343	0.47657
1400	0.54060	0.45940
1600	0.55386	0.44614
1800	0.56392	0.43608
2000	0.57138	0.42862
2200	0.57680	0.42320
2400	0.58059	0.41941
2600	0.58308	0.41692
2800	0.58452	0.41548
3000	0.58512	0.41488
3200	0.58502	0.41498
3400	0.58432	0.41568
3600	0.58321	0.41679
3800	0.58169	0.41831
4000	0.57985	0.42015
4200	0.57776	0.42224
4400	0.57546	0.42454
4600	0.57302	0.42698
4800	0.57047	0.42953
5000	0.56784	0.43216
5400	0.56248	0.43752
5800	0.55712	0.44288
6000	0.55449	0.44551

Table 11

Gas-ThO$_2$ Interface Spectral Hemispherical Properties (medium 1-Gas ; medium 2-ThO$_2$)

Wavelength λ (μ)	$\alpha_{\lambda 12}$	$\rho_{\lambda 11}$
0.20	0.82430	0.17570
0.25	0.82442	0.17558
0.30	0.82455	0.17545
0.35	0.82455	0.17545
0.40	0.82468	0.17532
0.45	0.82480	0.17520
0.50	0.82480	0.17520
0.55	0.82480	0.17520
0.60	0.82493	0.17507
0.65	0.82493	0.17503
0.70	0.82493	0.17503
0.75	0.82506	0.17494
0.80	0.82506	0.17404
0.85	0.82506	0.17404
0.90	0.82506	0.17404
0.95	0.82518	0.17482
1.00	0.82518	0.17482
1.05	0.82518	0.17482
1.10	0.82518	0.17482
1.15	0.82518	0.17482
1.20	0.82518	0.17482
1.25	0.82518	0.17482

Table 11 (Cont'd)

Wavelength λ (μ)	$\alpha_{\lambda 12}$	$\rho_{\lambda 11}$
1.30	0.82518	0.17482
1.35	0.82518	0.17482
1.40	0.82518	0.17482
1.45	0.82531	0.17469
1.50	0.82531	0.17469
2.00	0.82556	0.17444
2.50	0.82569	0.17431
3.00	0.82569	0.17431
3.50	0.82582	0.17418
4.00	0.82594	0.17406
4.50	0.82594	0.17406
5.00	0.82607	0.17393
5.50	0.82607	0.17393
6.00	0.82620	0.17380
6.50	0.82620	0.17380
7.00	0.82632	0.17368
7.50	0.82632	0.17368
8.00	0.82645	0.17355
8.50	0.82658	0.17342
9.00	0.82670	0.17330
9.50	0.82670	0.17330
10.00	0.82670	0.17330

Table 12

Gas-ThO$_2$ Interface Total Hemispherical Properties (medium 1-Gas ; medium 2-ThO$_2$)

Temperature (°K)	α_{12}	ρ_{11}
1200	0.82588	0.17412
1400	0.82578	0.17422
1600	0.82570	0.17430
1800	0.82563	0.17437
2000	0.82556	0.17444
2200	0.82551	0.17449
2400	0.82546	0.17454
2600	0.82542	0.17458
2800	0.82538	0.17462
3000	0.82534	0.17466
3200	0.82531	0.17469
3400	0.82527	0.17473
3600	0.82524	0.17476
3800	0.82522	0.17478
4000	0.82519	0.17481
4200	0.82517	0.17483
4400	0.82514	0.17486
4600	0.82512	0.17488
4800	0.82510	0.17490
5000	0.82508	0.17492
5400	0.82504	0.17496
5800	0.82500	0.17500
6000	0.82499	0.17501

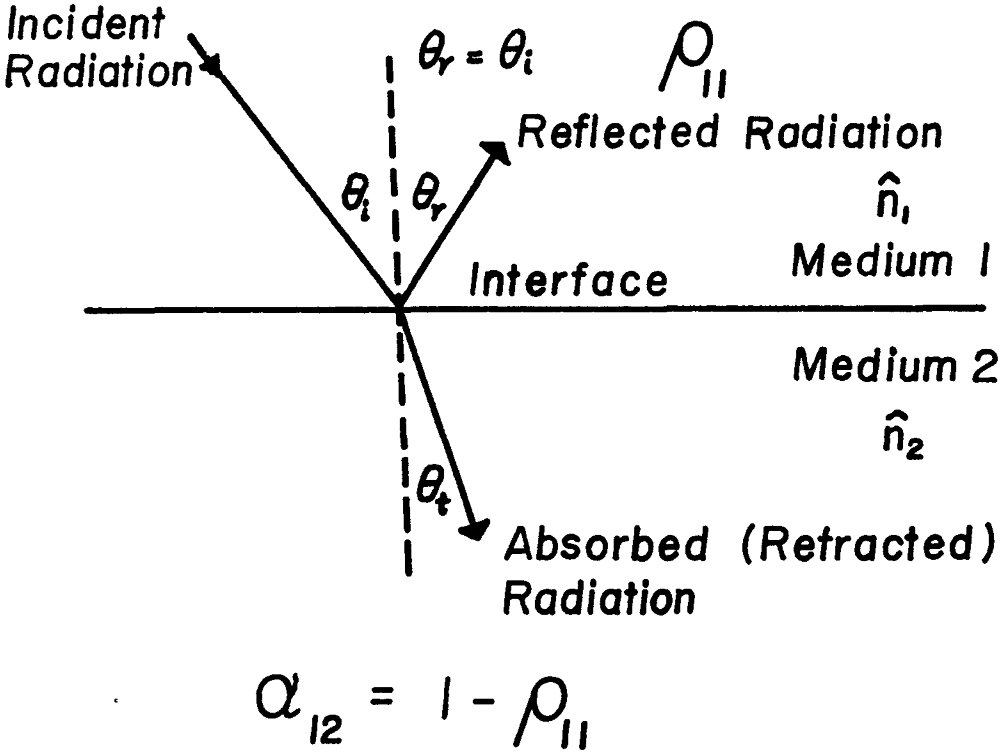

Fig. 1 Incident, reflected and refracted radiation at Interface

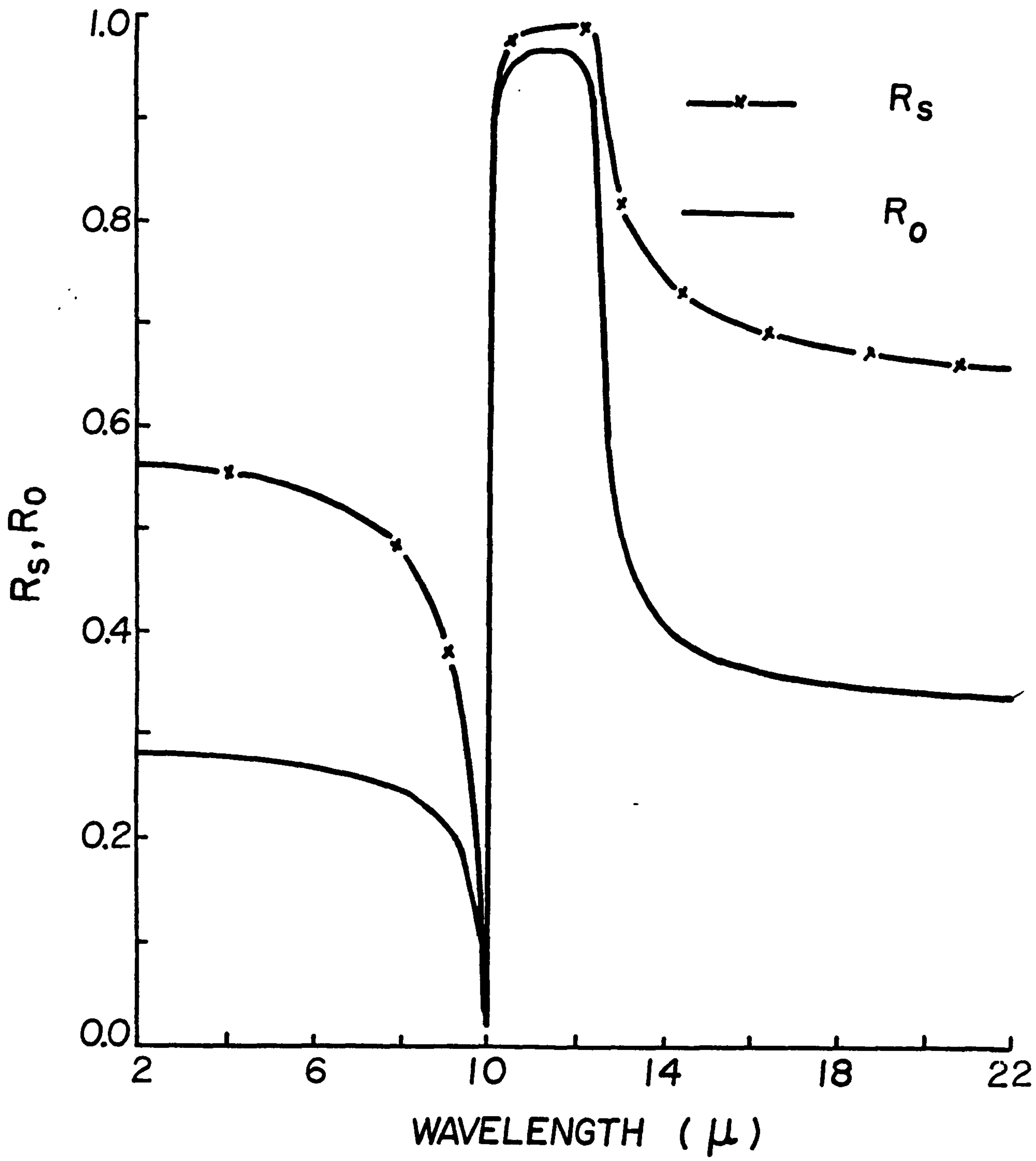

Fig. 2 Reflectance spectra of the Lorentz oscillator for the incidence angle $\theta = 70^\circ$; polarization $\alpha = 0$.

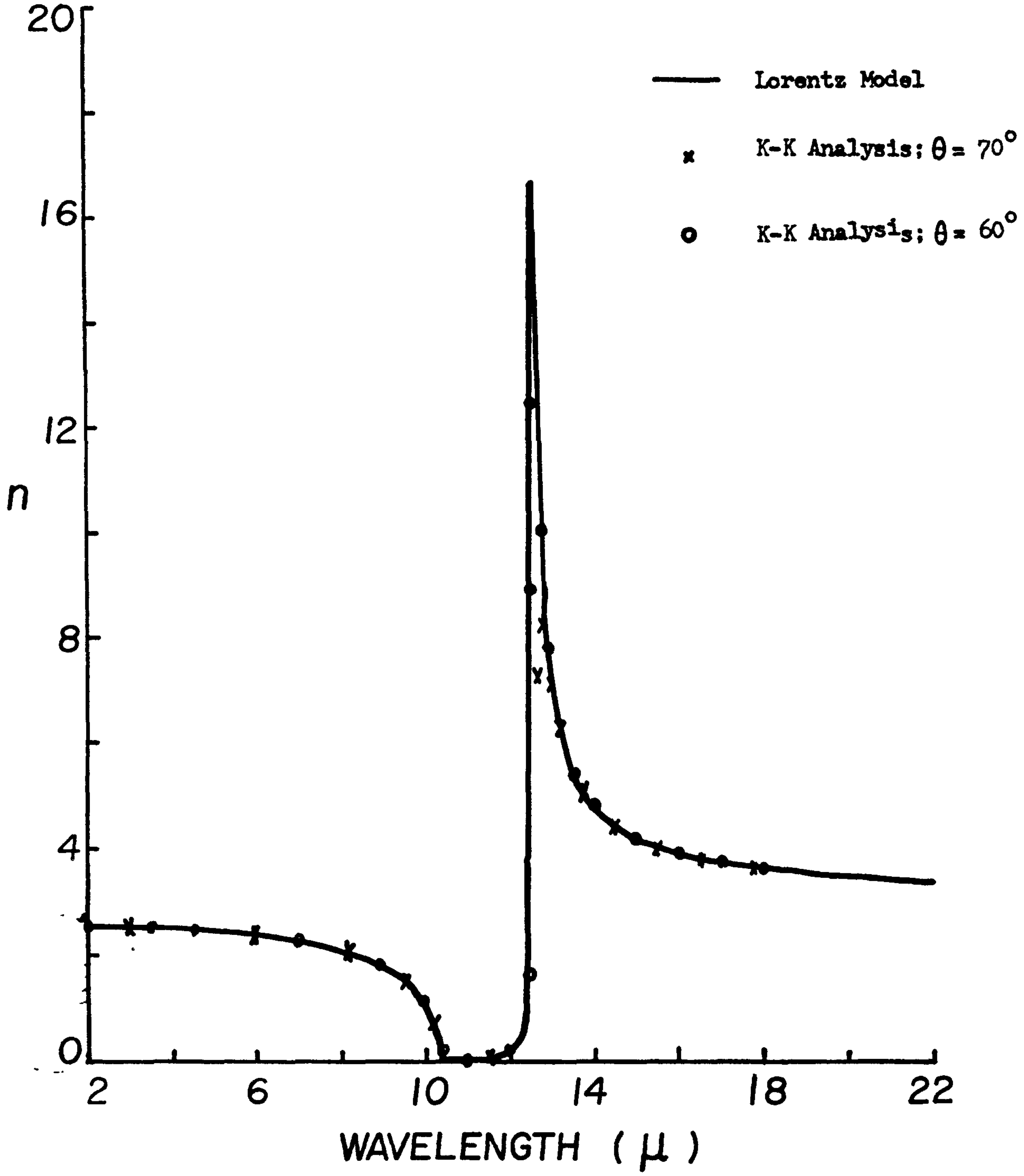

Fig. 3 Index of Refraction by Iterative K-K analysis compare with the values from Lorentz oscillator.

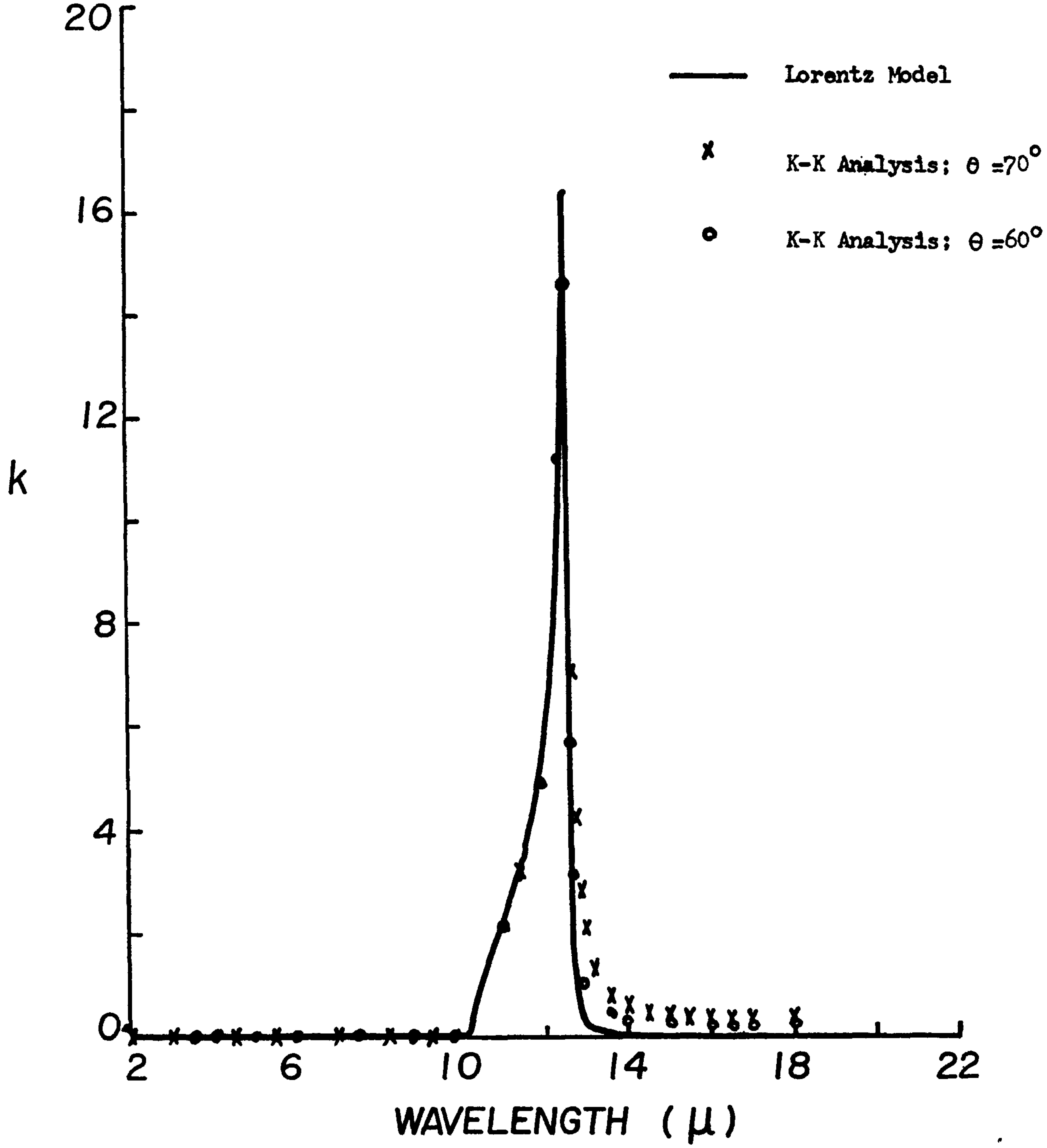

Fig. 4 Extinction Coefficient by Iterative K-K analysis compare with the values from Lorentz oscillator.

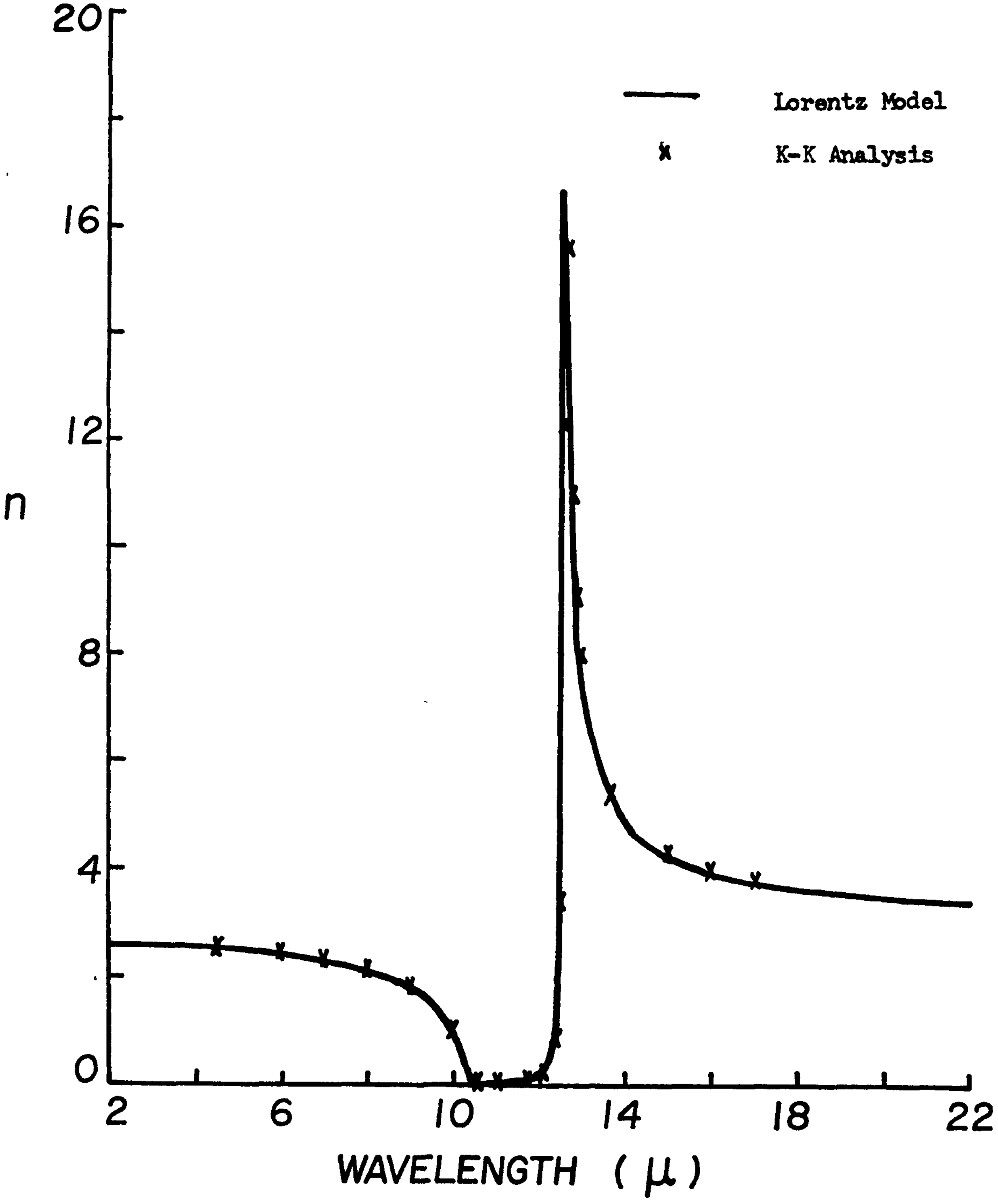

Fig. 5 Index of Refraction from the values of Extinction Coefficient with K-K analysis.

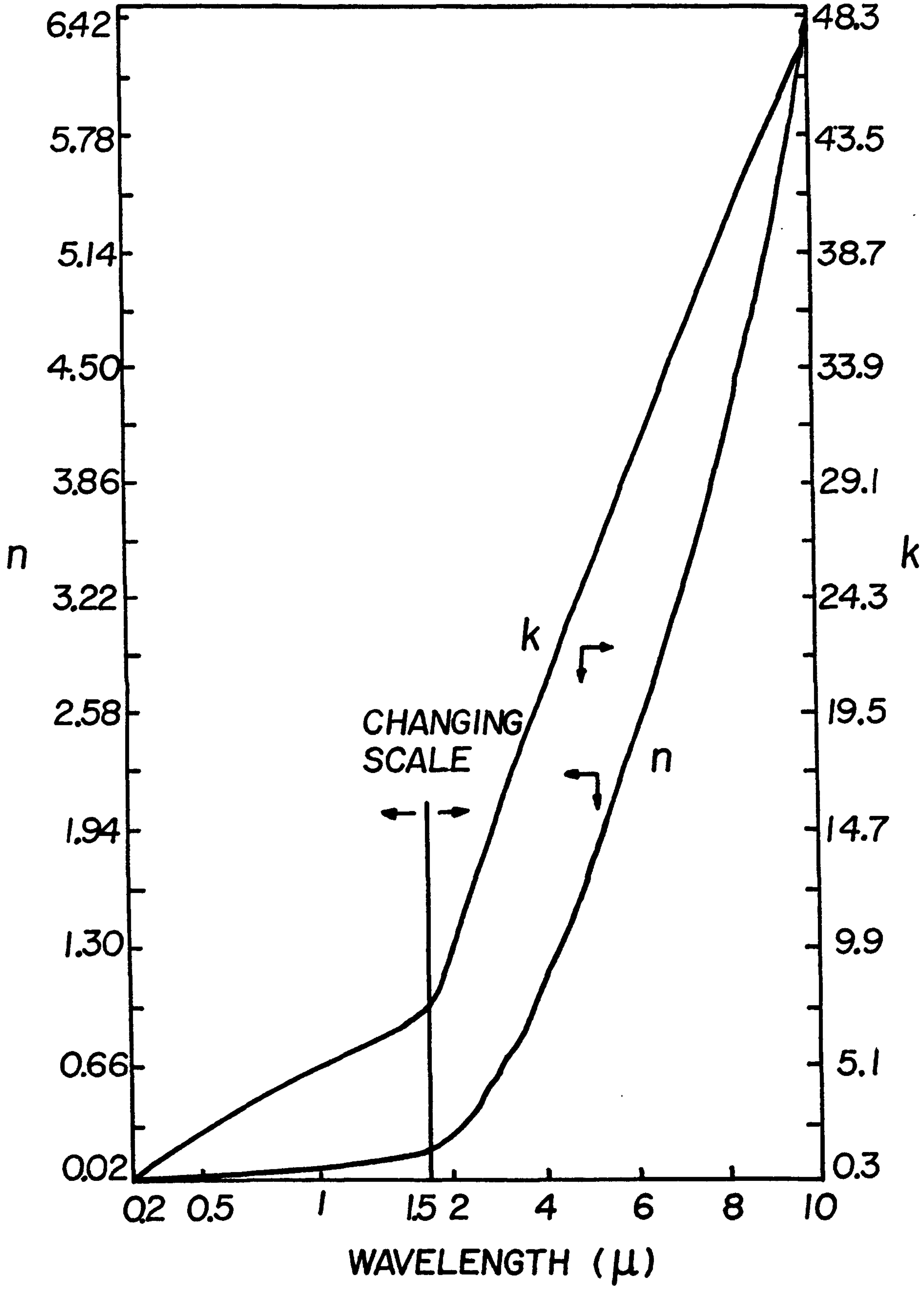

Fig. 6 Optical Constants of Sodium at Various Wavelength.

(From Ref. 5)

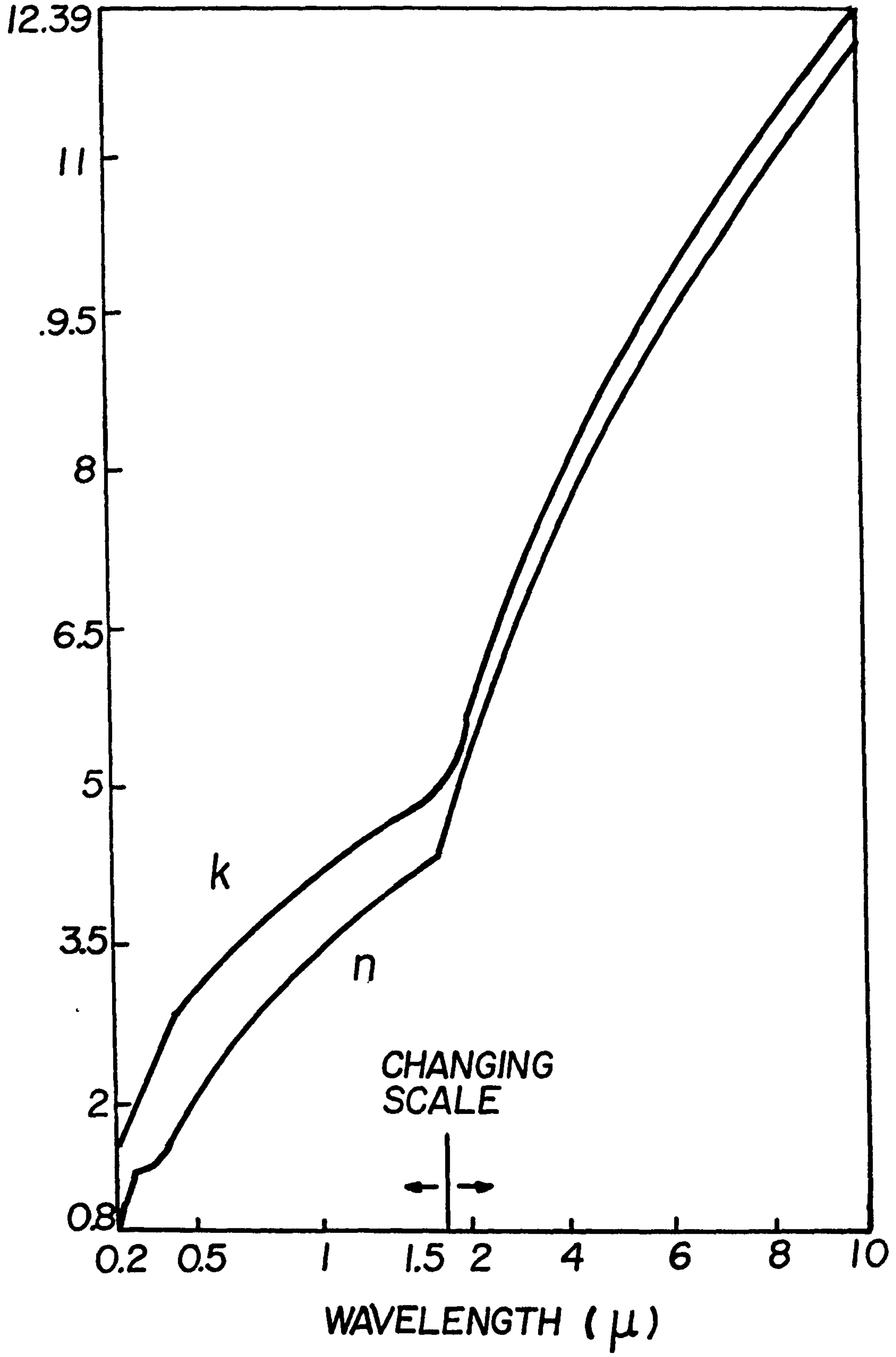

Fig. 7 Optical Constants of Steel at Various Wavelength

(From Ref. 5)

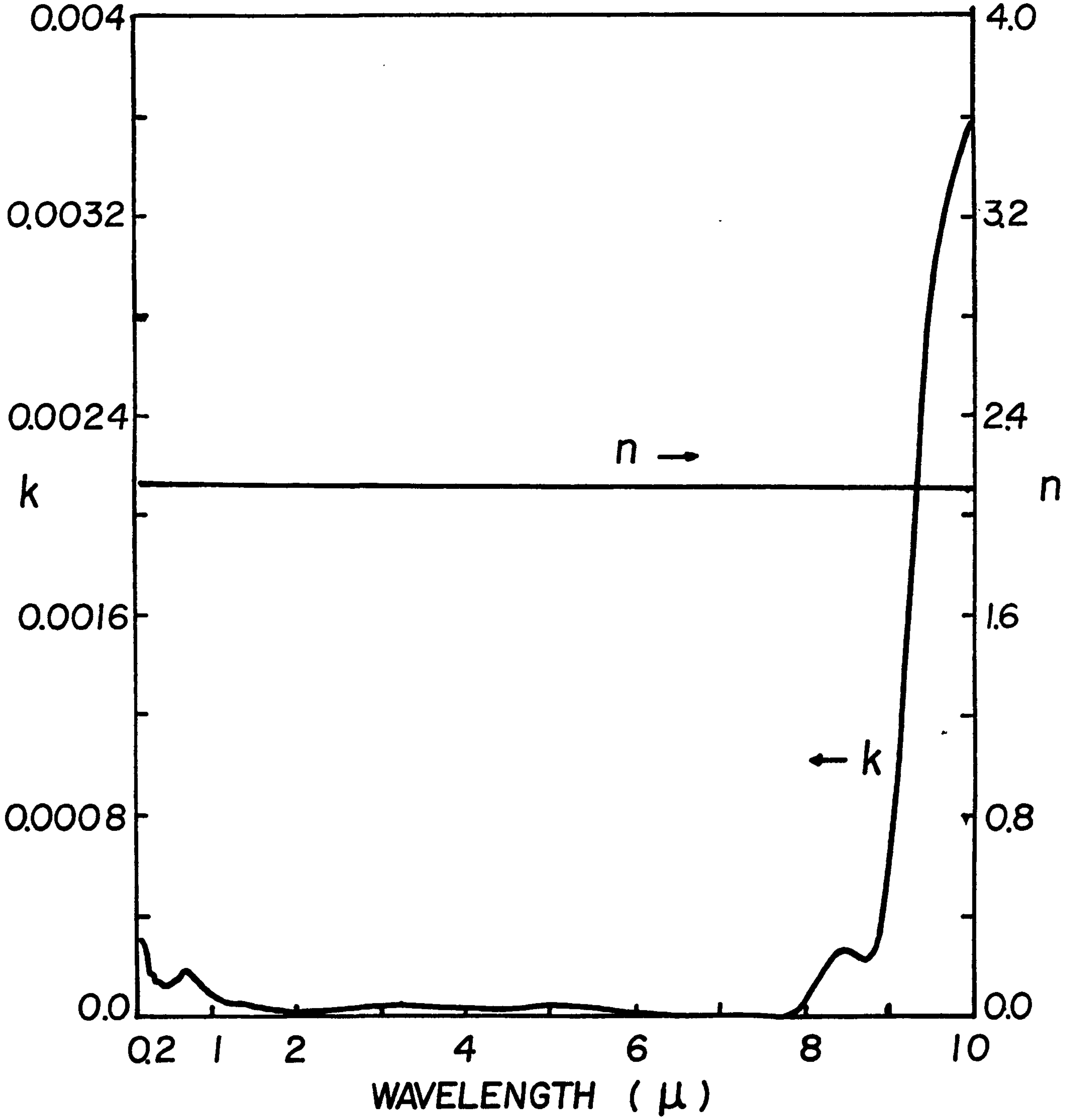

Fig. 8 Optical Constants of ThO_2 at Various Wavelengths

Based on the data of Table 4

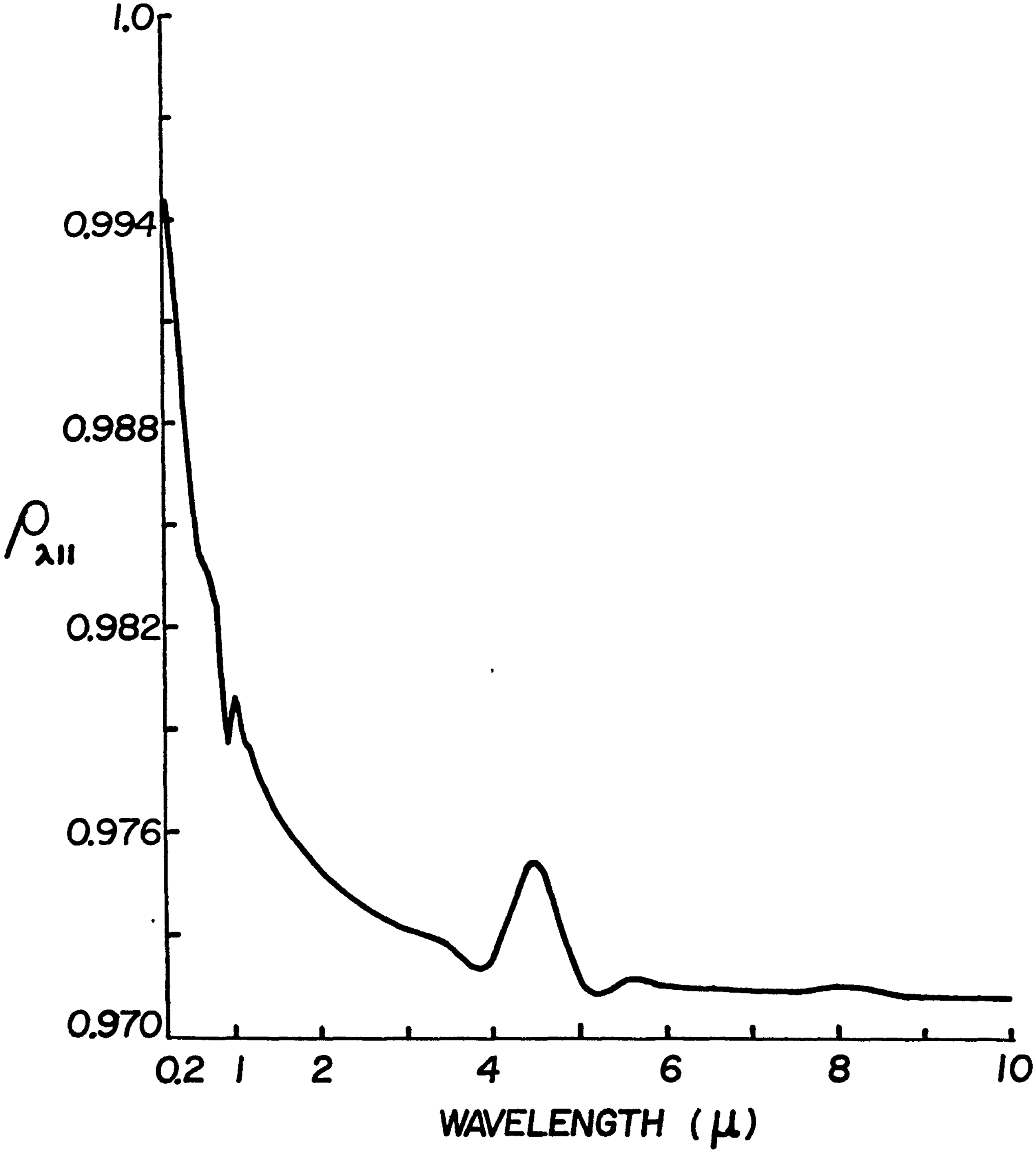

Fig. 9 ThO_2-Sodium Interface Spectral Hemispherical Reflectance

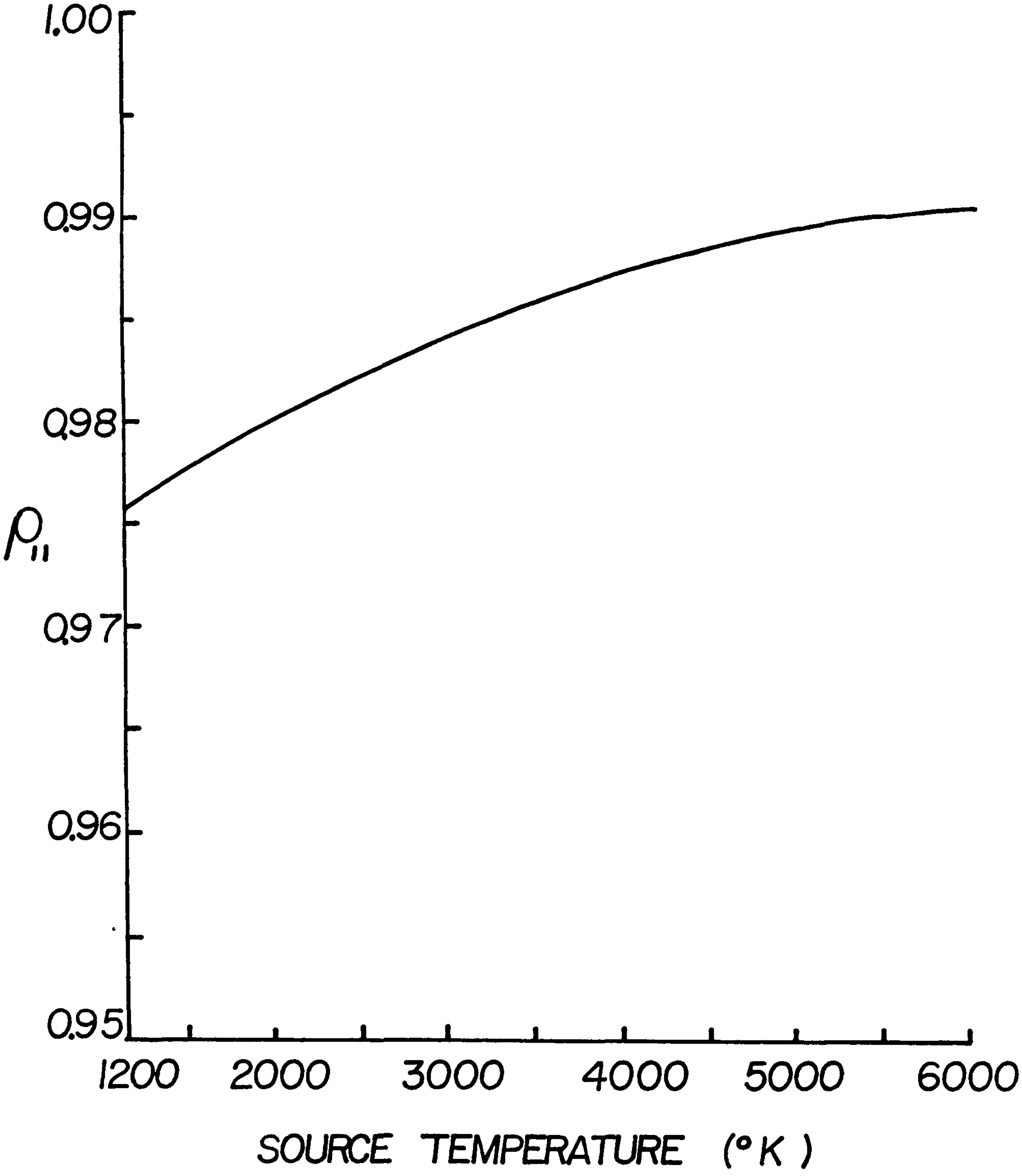

Fig. 10 ThO_2-Sodium Interface Total Hemispherical Reflectance

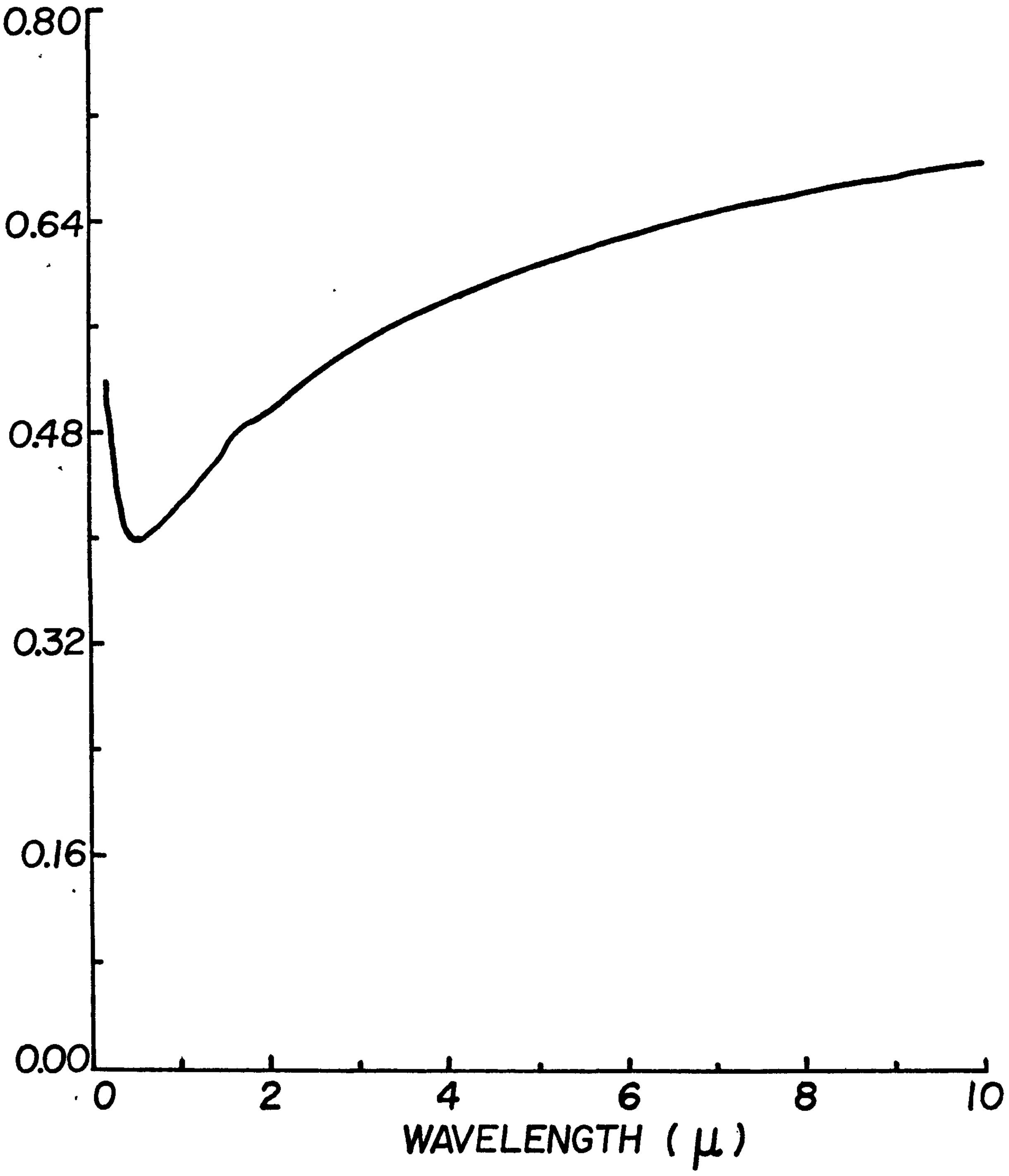

Fig. 11 ThO_2-Steel Interface Spectral Hemispherical Reflectance

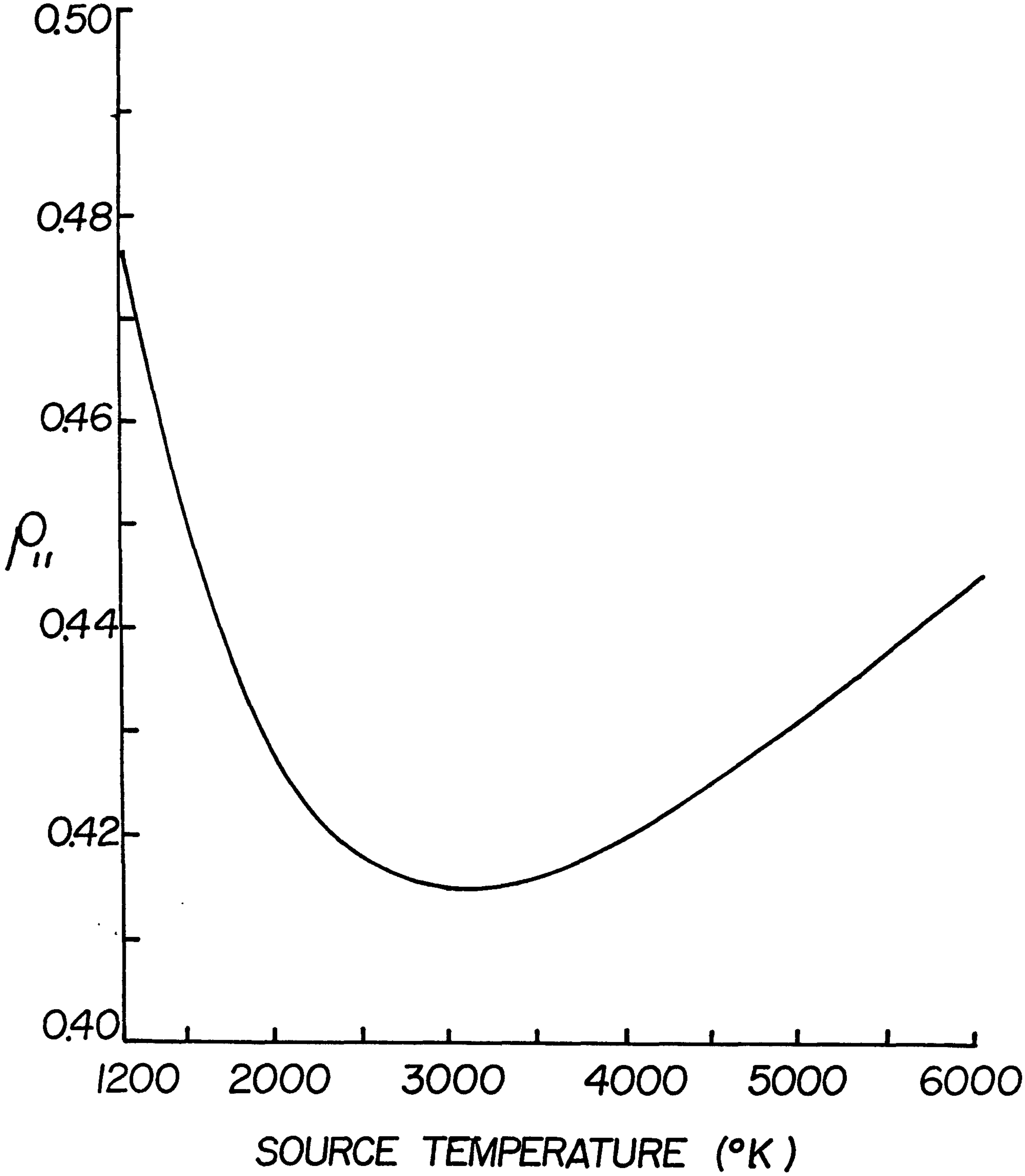

Fig. 12 ThO_2-Steel Interface Total Hemispherical Reflectance

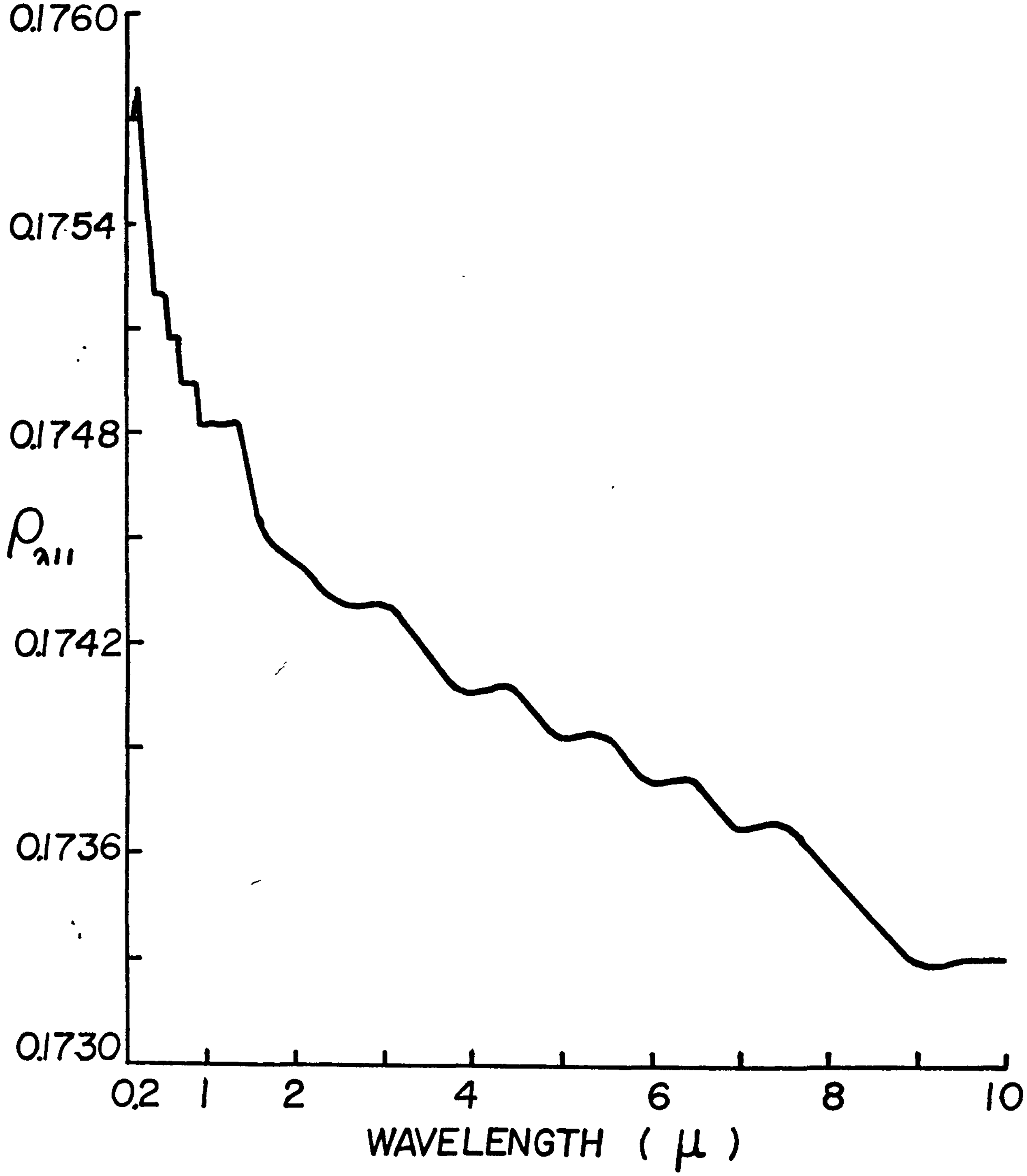

Fig. 13 Gas-ThO_2 Interface Spectral Hemispherical Reflectance

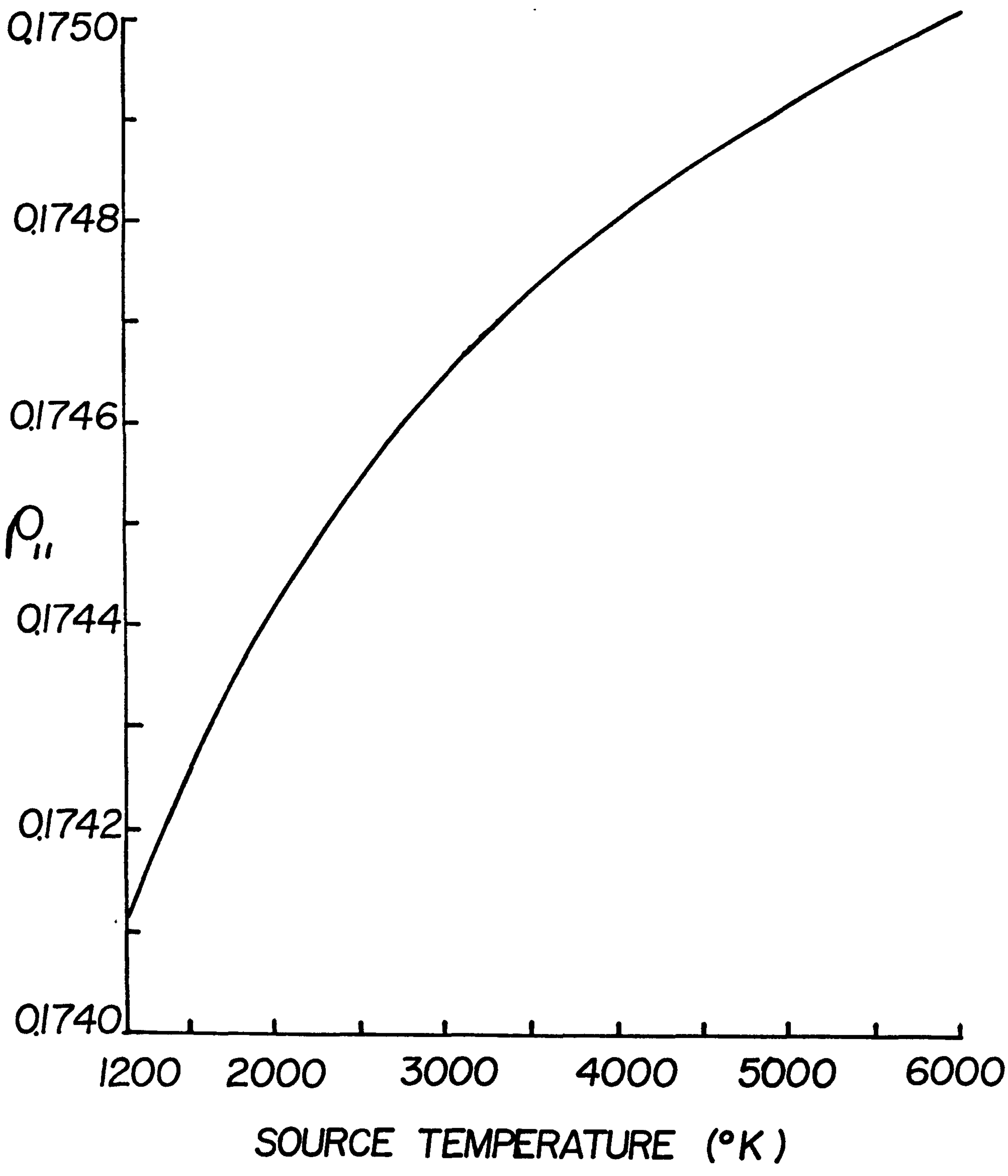

Fig. 14 Gas-ThO_2 Interface Total Hemispherical Reflectance

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APPENDIX A

LORENTZ OSCILLATOR (SEE REF. 13, pp. 42-45)

Consider an atom with electrons bound to the nucleus in much the same way as a small mass can be bound to a large mass by a spring. The motion of an electron bound to the nucleus can be represented by,

$$m\frac{d^2r}{dt^2} + m\gamma\frac{dr}{dt} + ma^2r = -eE_{loc} \qquad (A.1)$$

electronic acceleration force	viscous damping force	Hooke's restoring force	electric force

where: m - electronic mass

e - magnitude of electronic charge

a - resonance frequency

γ - damping constant

r - displacement of electron

E_{loc} - local microscopic electric field acting on the electron

The local field can be taken to vary in time as $e^{i\omega t}$. Thus, the solution to Eq. (A.1) is

$$\hat{r} = \frac{-eE_{loc}/m}{(a^2-\omega^2) - i\gamma\omega} \qquad (A.2)$$

The induced dipole moment is

$$\hat{p} = \frac{e^2E_{loc}/m}{(a^2-\omega^2) - i\gamma\omega} \qquad (A.3)$$

Note that it is important to be consistent in the form of the time variation in the electric field with the definition of the complex refractive index. The use of a time variation $e^{i\omega t}$ leads to a complex refractive index $\hat{n} = n-ik$, and $e^{-i\omega t}$ leads to $\hat{n} = n+ik$.

Assume a linear relationship exists between $\hat{p}$ and E_{loc} if the displacement r is sufficiently small,

$$\hat{p} = \hat{\alpha}(\omega)E_{loc} \tag{A.4}$$

where $\hat{\alpha}(\omega)$ is frequency-dependent atomic polarizability, and for a one-electron atom,

$$\hat{\alpha}(\omega) = (e^2/m)/\left[(a^2-\omega^2)+i\gamma\omega\right] \tag{A.5}$$

For N one-electron atoms per unit volume, the macroscopic polarization is

$$P = N\hat{p} = N\hat{\alpha}(\omega)\ E_{loc} \tag{A.6}$$

Preceeding with the assumption the microscopic electric field E_{loc} can be approximated by the macroscopic field E, we have

$$P = N\hat{\alpha}(\omega)E = X_e E \tag{A.7}$$

X_e is macroscopic electric susceptibility.

Define a complex displacement $\hat{D}$ such that

$$\hat{D} = \hat{\varepsilon}E = \varepsilon_o E + 4\pi P \tag{A.8}$$

From Eqs. (A.7) and (A.8), the dielectric function $\hat{\varepsilon}(=\varepsilon_1+i\varepsilon_2)$ is

$$\hat{\varepsilon} = \varepsilon_o + 4\pi N\hat{\alpha}(\omega) \tag{A.9}$$

Thus,

$$\hat{\varepsilon} = \varepsilon_o + \frac{4\pi Ne^2}{m}\frac{1}{(a^2-\omega^2)+i\gamma\omega} \tag{A.10}$$

From Maxwell's equations

$$\varepsilon_1 = (n^2-k^2)/\mu \tag{A.11}$$

$$\varepsilon_2 = 2nk/\mu = 4\pi\sigma/\omega \tag{A.12}$$

μ: magnetic permeability. σ: conductivity. For non-magnetic materials, μ is equal to unity. We can find

$$\mathcal{E}_1 = n^2 - k^2 = \mathcal{E}_o + \frac{4\pi Ne^2}{m}\,\frac{(a^2-\omega^2)}{(a^2-\omega^2)+\gamma^2\omega^2} \qquad (A.13)$$

$$\mathcal{E}_2 = 2nk = -\frac{4\ Ne^2}{m}\,\frac{\gamma\omega}{(a^2-\omega^2)^2+\gamma^2\omega^2} \qquad (A.14)$$

Again, from Eqs. (A.11) and (A.12), we find that for non-magnetic materials

$$n = \left\{\tfrac{1}{2}\left[(\mathcal{E}_1^2 + \mathcal{E}_2^2)^{\frac{1}{2}} + \mathcal{E}_1\right]\right\}^{\frac{1}{2}} \qquad (A.15)$$

$$k = \left\{\tfrac{1}{2}\left[(\mathcal{E}_1^2 + \mathcal{E}_2^2)^{\frac{1}{2}} - \mathcal{E}_1\right]\right\}^{\frac{1}{2}} \qquad (A.16)$$

Summary

Equations (A.13) and (A.14) can be cast into dimensionless form. Then the susceptibility X_e and conductivity   in the neighborhood of a resonance frequency a are given by

$$X_e = \rho'\,\frac{1-\nu^2}{(1-\nu^2)^2+\gamma^2\nu^2} \qquad (A.17)$$

and

$$(\sigma'/\nu') = -\,2\pi\rho'\,\frac{\gamma'\nu'}{(1-\nu^2)^2+\gamma^2\nu^2} \qquad (A.18)$$

where: ν' - is the measured frequency divided by a.

σ' - is the conductivity divided by a.

γ' - is called the width of the resonance.

ρ' - is given by $Ne^2/4\pi^2ma^2$ which is strength of the resonance.

And n, k can be written alternatively as

$$n^2 = \tfrac{1}{2}\left\{\left[\varepsilon^2 + 4(\sigma/\nu)^2\right]^{\frac{1}{2}} + \varepsilon\right\} \qquad \text{(A.19)}$$

$$k^2 = \tfrac{1}{2}\left\{\left[\varepsilon^2 + 4(\sigma/\nu)^2 \, {}^{\frac{1}{2}} - \varepsilon\right\} \qquad \text{(A.20)}$$

respectively, where

$$\varepsilon = \varepsilon_o + 4\pi X_e \qquad \text{(A.21)}$$

A.1 Criteria in Determining the Parameters of the Lorentz Model

In order to obtain a theoretical fit of Eqs. (A.17) and (A.18) to experimental data, the use of the following principles can be helpful:

a. The initial choice of a should correspond to the steepest point on the long wavelength side of the reflection peak. Alternatively one should use Havelock's[21] formula

$$a = \nu_{\max}\left(1 + \frac{n_+^2 - n_-^2}{6n_-^2 - 4}\right)^{\frac{1}{2}}$$

where: $\nu_{\max}$ is frequency at the reflectivity maximum, n_+ and n_- are the limiting indice of refraction at long and short wavelength, respectively.

b. The initial choice of ε_o should give the observed limiting reflectivity at short wavelength according to the formula

$$R_{\nu\to\infty} = \left(\frac{\varepsilon_o^{\frac{1}{2}} - 1}{\varepsilon_o^{\frac{1}{2}} - 1}\right)^2$$

c. The initial choice of ρ should give the correct reflectivity on the long wavelength side of the band. It may be chosen to give the static electric constant according to the formulas (A.17) and (A.21) by taking the limit $\nu\to 0$.

d. The initial choice of γ is governed by the maximum reflectivity. The approximation

$$\max R \sim 1 - (\gamma/\pi\rho)$$

is rough but very useful.

Repeat with the process a to d , we can determine the values of these parameters by trial and error until the best fit is reached. Therefore, a theoretical spectrum of R_o can be calculated. In fact, with very limiting cases the theoretical curve can succeed in aligning with the experimental curve.

APPENDIX B

REFLECTANCE AND PHASE-SHIFT DISPERSION RELATION (REF. 13, pp. 244-248)

The derivation of the phase-shift dispersion relation requires that the complex reflectivity amplitude $\hat{r}(\omega)$ be analytically continued into the complex frequency plane. Suppose that $\hat{r}(\omega)$ and hence $\ln\hat{r}(\omega)$ can be analytically continued into the upper half of the complex frequency plane, which we denote as domain D. A contour integral as indicated in Fig. B.1 then yields the desired dispersion relation.

The linear causal relation between $E_r(\omega)$ and $E_i(\omega)$ require analyticity of $r(\omega)$ in the domain D as shown by the following:

$$E_r(t) = \int_{-\infty}^{\infty} E_r(\omega)\, e^{-i\omega t}\, d\omega \tag{B.1}$$

$$E_r(\omega) = \hat{r}(\omega)\, E_i(\omega) \tag{B.2}$$

$$E_i(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} E_i(t')\exp(i\omega t')\, dt' \tag{B.3}$$

By substituting Eqs. (B.2) and (B.3) into Eq. (B.1), it yields

$$E_r(t) = \int_{-\infty}^{\infty} G(t-t')\, E_i(t')\, dt' \tag{B.4}$$

where:

$$G(t-t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} \hat{r}(\omega)\, \exp\left[-i\omega(t-t')\right]\, d\omega \tag{B.5}$$

which is the Fourier transform of $\hat{r}(\omega)$. If this transform can be inverted, then,

$$\hat{r}(\omega) = \int_{-\infty}^{\infty} G(T)e^{i\omega t}\, dT \quad ; \quad T \equiv t-t' \tag{B.6}$$

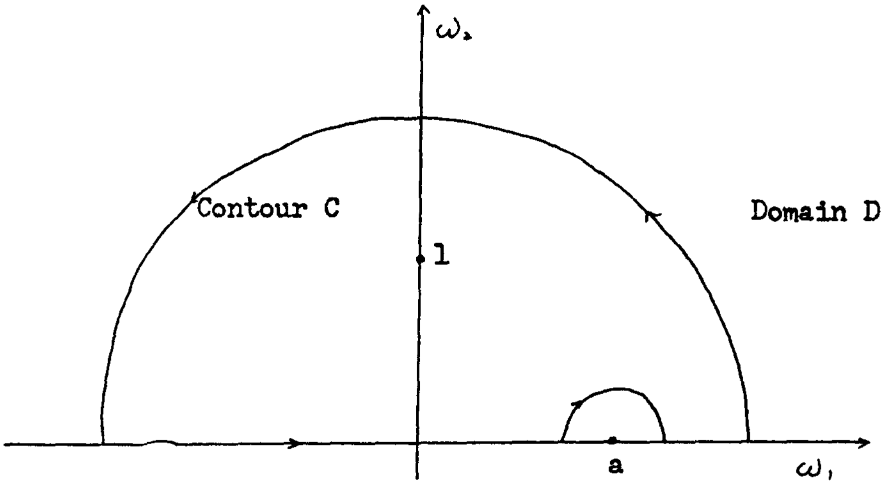


Fig. B.1 Integration Contour in Complex Frequency Plane $\hat{\omega} = \omega_1 + i\omega_2$

We want to derive a dispersion relation for $\mathrm{In}\hat{r}(\hat{\omega})$, i.e., we want an integral relationship between $\mathrm{In}\rho(\omega)$ and $\theta(\omega)$ so we can eleminate one of the unknowns in the equation

$$\mathrm{In}\hat{r}(\omega) = \mathrm{In}\rho(\omega) + i\theta(\omega) \tag{B.7}$$

Therefore, a function other than $\mathrm{In}\hat{r}(\hat{\omega})$ must be used for the integration over the contour shown in Fig. B.1. The function

$$f(\hat{\omega}) = (1+a\hat{\omega})\mathrm{In}\ \hat{r}(\hat{\omega})/\left[(1+\hat{\omega}^2)(a-\hat{\omega})\right] \tag{B.8}$$

which can be integrated over the contour C satisfies the dispersion relation for $\mathrm{In}\hat{r}(\hat{\omega})$.

Integrating Eq. (B.8), we have

$$\int_C \frac{(1+a\hat{\omega})\ \mathrm{In}\left[\hat{r}(\hat{\omega})\right]}{(1+\hat{\omega}^2)(a-\hat{\omega})} d\hat{\omega} = 2\pi i \sum_j \mathrm{Res}(\hat{\omega}_j) \tag{B.9}$$

This becomes

$$\text{p.v.} \int_{-\infty}^{\infty} \frac{(1+a\omega)\ \mathrm{In}\left[\hat{r}(\hat{\omega})\right]}{(1+\omega^2)(a-\omega)} d\omega + i\pi \mathrm{In}\left[\hat{r}(a)\right] = i\pi\mathrm{In}\left[r(i)\right] \tag{B.10}$$

since the only pole enclosed by the contour is $\hat{\omega}=i$, and the only pole on the contour is $\hat{\omega}=a$. From Eq. (B.6), we see $\hat{r}(i)$ is real, so is $\mathrm{In}[\hat{r}(i)]$. Substituting Eq. (B.7) into (B.10) and equating the real parts of the resulting equation, we find

$$\phi(a) = \frac{1}{\pi}\,\text{p.v.}\int_{-\infty}^{\infty} \frac{1+a\omega}{1+\omega^2}\,\mathrm{In}[\rho(\omega)]\,\frac{d\omega}{a-\omega} \tag{B.11}$$

Using Eq. (B.2), we see that the complex conjugate of r is

$$\hat{r}^*(\omega) = E_r^*(\omega)/E_i^*(\omega) = E_r(-\omega)/E_i(-\omega) \tag{B.12}$$

so $\hat{r}^*(\omega) = \hat{r}(-\omega)$ (B.13)

and $\mathrm{In}[\rho(\omega)] = \mathrm{In}[\rho(-\omega)]$ (B.14)

Considering integration of Eq. (B.11) over negative frequencies and using Eq. (B.14), we have

$$\frac{1}{\pi}\,\text{p.v.}\int_{-\infty}^{0} \frac{(1+a\omega)\ \mathrm{In}\rho(\omega)}{(1+\omega^2)(a-\omega)}\,d\omega = \frac{1}{\pi}\,\text{p.v.}\int_{0}^{\infty} \frac{(1-a\omega)\ \mathrm{In}\rho(\omega)}{(1+\omega^2)(a+\omega)}\,d\omega \tag{B.15}$$

Therefore, Eq. (B.11) becomes

$$\phi(a) = \frac{2a}{\pi}\,\text{p.v.}\int_{0}^{\infty} \frac{\mathrm{In}\rho(\omega)}{a^2-\omega^2}\,d\omega \tag{B.16}$$

The singularity at $\omega=a$ is removed by subtracting

$$\frac{2a}{\pi}\,\text{p.v.}\int_{0}^{\infty} \frac{\mathrm{In}\rho(a)}{a^2-\omega^2}\,d\omega = 0 \tag{B.17}$$

from Eq. (B.16). Then from the normal reflectivity relation

$$R(\omega) = \hat{r}(\omega)\hat{r}^*(\omega) = \rho^2 \tag{B.18}$$

we obtain the desired dispersion relation

$$\phi(a) = \frac{a}{\pi}\int_{0}^{\infty} \frac{\mathrm{In}[R(\omega)/R(a)]}{a^2-\omega^2}\,d\omega \tag{B.19}$$

There are several notable features of Eq. (B.19). A fractional error in reflectance, that is, a measurement which yields the same percentage error in reflectance at all frequencies, does not affect the phase. Such errors still yield the correct reflectance ratio $R(\omega)/R(a)$, and no effect to the phase at $\omega=a$.

APPENDIX C

NUMERICAL INTEGRATION OF THE PHASE-SHIFT EQUATION

The phase-shift equation,

$$\phi(a) = -\frac{2a}{\pi}\int_0^{\infty}\frac{\mathrm{In}\ R_s^{\frac{1}{2}}(\omega)}{\omega^2 - a^2}\,d\omega \qquad (C.1)$$

can be written, after integrating by parts, as

$$\phi(a) = \frac{1}{\pi}\int_0^{\infty}\mathrm{In}\left|\frac{\omega-a}{\omega+a}\right|\frac{d\,\mathrm{In}\ R_s^{\frac{1}{2}}(\omega)}{d\omega}\,d\omega \qquad (C.2)$$

To integrate by part one more time, let us choose

$$u = d\ \mathrm{In}\ R_s^{\frac{1}{2}}(\omega)/\,d\omega \quad ; \quad dv = \Big\{\mathrm{In}|\omega-a| - \mathrm{In}(\omega+a)\Big\}\,d\omega$$

Then,

$$\phi(a) = \frac{1}{\pi}\left\{\frac{d\ \mathrm{In}R_s^{\frac{1}{2}}(\omega)}{d\omega}\Big[(\omega-a)\mathrm{In}|\omega-a| - (\omega+a)\mathrm{In}(\omega+a) + 2a\Big]\right\}_0^{\infty}$$

$$- \int_0^{\infty}\Big[(\omega-a)\mathrm{In}|\omega-a| - (\omega+a)\mathrm{In}(\omega+a) + 2a\Big]\frac{d^2\mathrm{In}R_s^{\frac{1}{2}}(\omega)}{d\omega^2}\,d\omega \qquad (C.3)$$

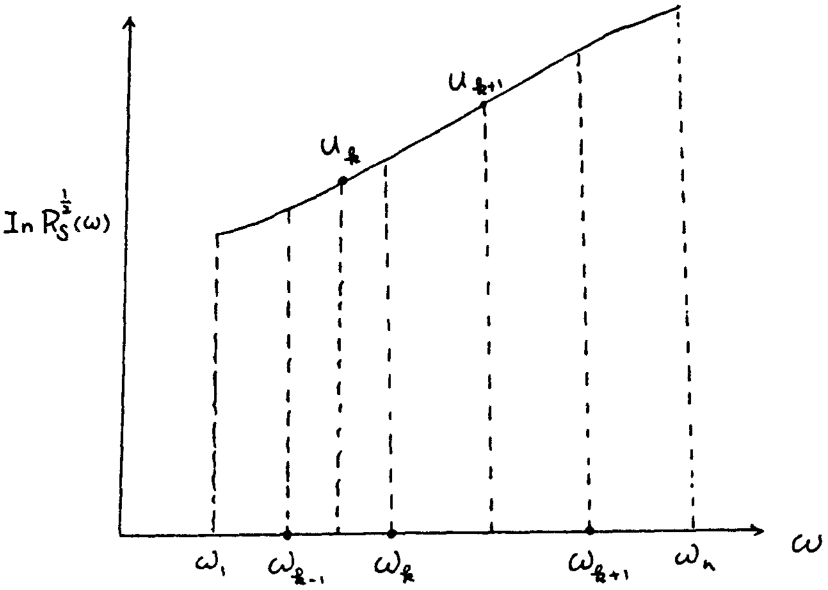
Because it is complex integral, we should use Cauchy principle value to simplify the integral to the desired form. Assume the slope of $R_s(\omega)$ is zero at $\omega=0$, and $\omega\to\infty$, the first term on the right hand side of Eq. (C.3) is then zero. Also for the last term in the integral,

$$\frac{2a}{\pi}\int_0^{\infty}\frac{d^2\,\mathrm{In}\ R_s^{\frac{1}{2}}(\omega)}{d\omega^2}\,d\omega \simeq 0 \qquad (C.4)$$

Thus, it is only left with

$$\phi(a) = \frac{1}{\pi}\int_0^{\infty}\Big((\omega+a)\mathrm{In}(\omega+a) + (a-\omega)\mathrm{In}|\omega-a|\Big)\frac{d^2\,\mathrm{In}\ R_s^{\frac{1}{2}}(\omega)}{d\omega^2}\,d\omega \qquad (C.5)$$

In reference to the sketch, let



$$u_k = \frac{\mathrm{In}\, R_s^{\frac{1}{2}}(\omega_k) - \mathrm{In}\, R_s^{\frac{1}{2}}(\omega_{k-1})}{\omega_k - \omega_{k-1}} \qquad \text{at } \frac{\omega_k + \omega_{k-1}}{2}$$

$$u_{k+1} = \frac{\mathrm{In}\, R_s^{\frac{1}{2}}(\omega_{k+1}) - \mathrm{In}\, R_s^{\frac{1}{2}}(\omega_k)}{\omega_{k+1} - \omega_k} \qquad \text{at } \frac{\omega_k + \omega_{k+1}}{2}$$

$$\frac{d^2 \mathrm{In}\, R_s^{\frac{1}{2}}(\omega)}{d\omega^2} d\omega = u_{k+1} - u_k = \gamma_k$$

Therefore,

$$\phi(a) = \frac{1}{\pi} \sum_{k=2}^{n-1} \gamma_k \Big((\omega+a)\mathrm{In}(\omega+a) + (a-\omega)\mathrm{In}|\omega-a| \Big) \qquad \text{(C.6)}$$

In using this formula it is essential to impose the first two values (k=1, 2) of $R_s(\omega)$ be the same. So are the last two values (k=n-1, n) because of the assumption imposed.

APPENDIX D

Optical Density of Single Crystal ThO_2 From Bates' Report (Ref. 16)

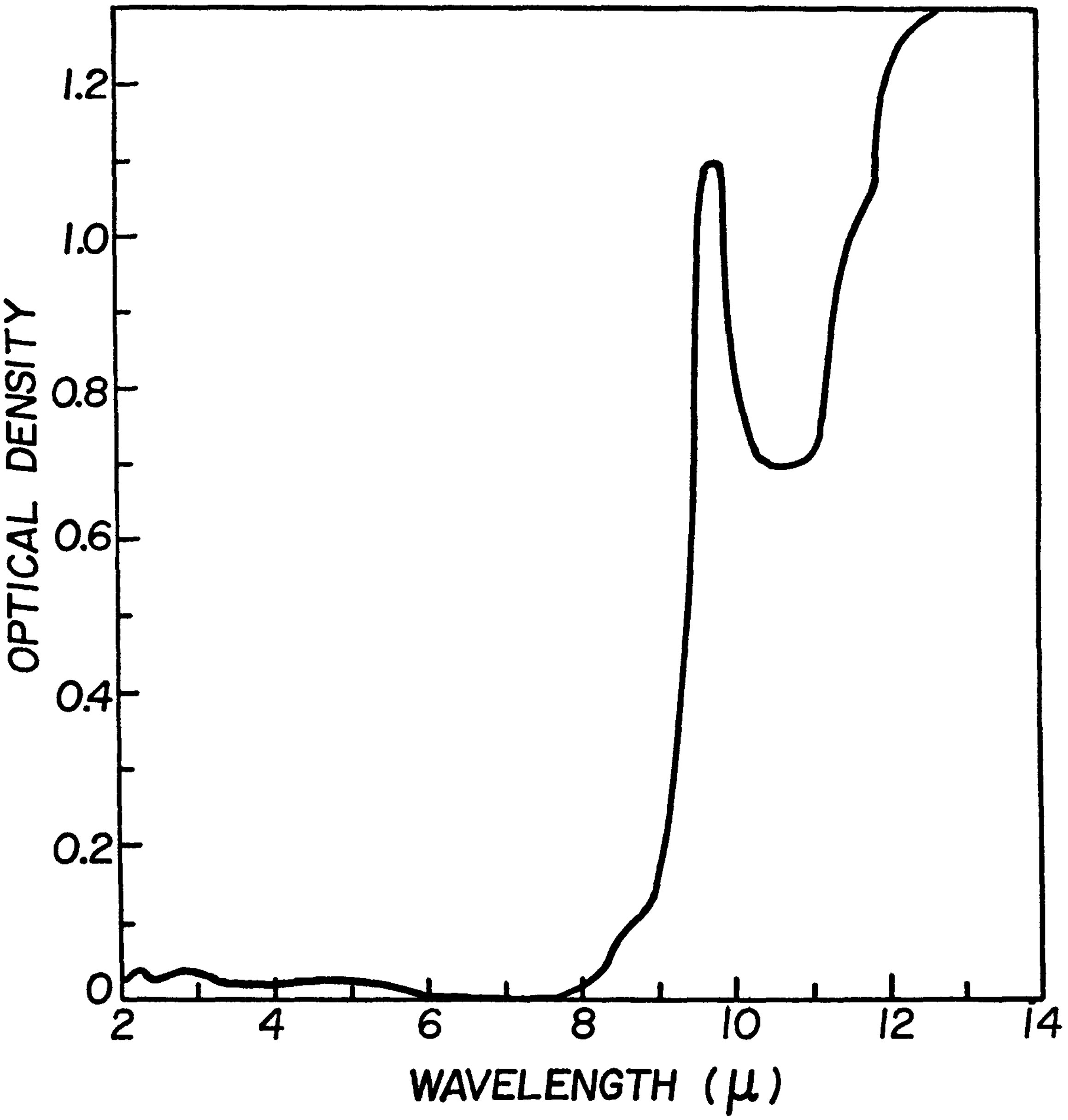


Fig. D.1 Infrared Absorption Spectrum of Single Crystal ThO_2

(Sample Thickness is 0.048 cm)

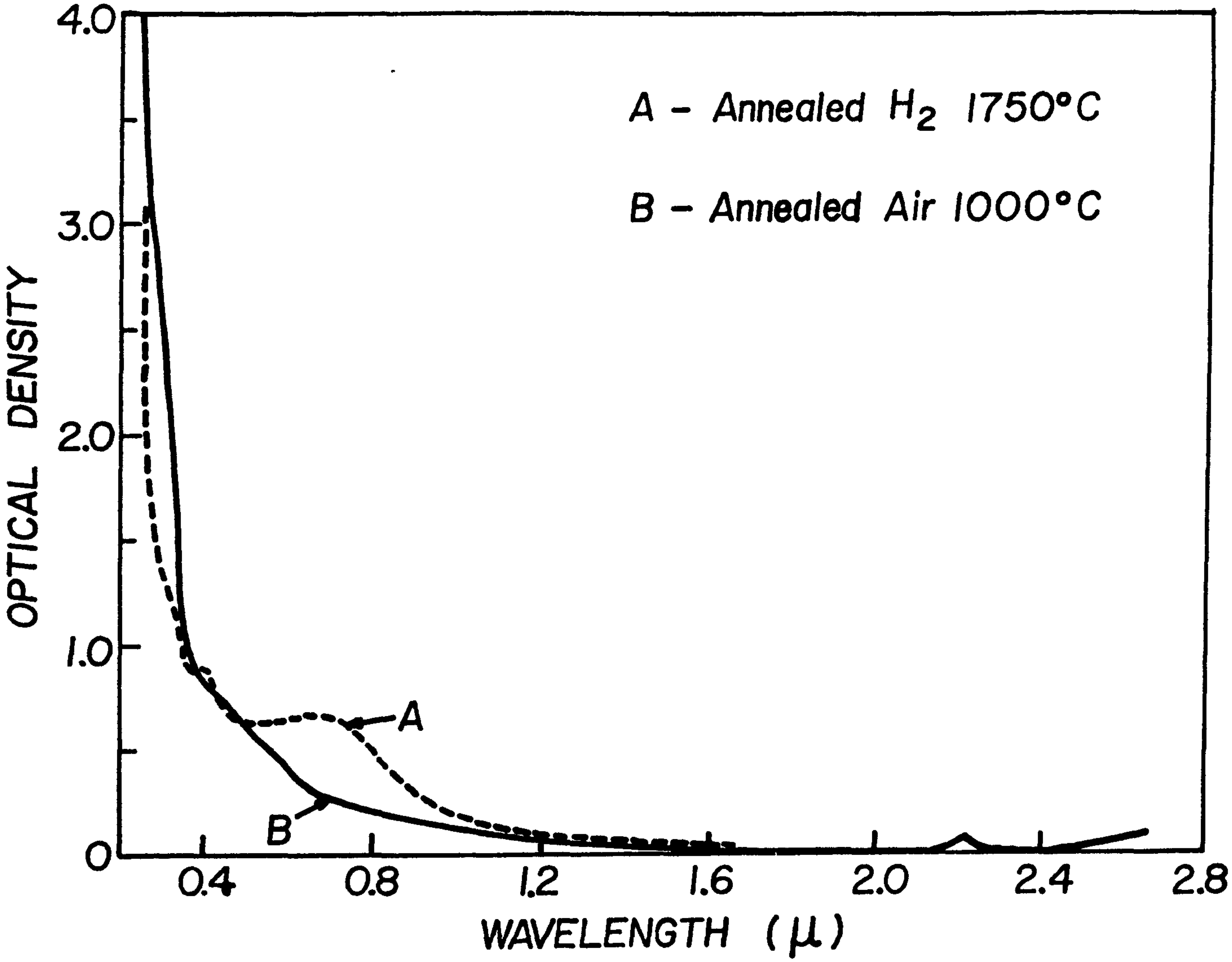


Fig. D.2 Ultraviolet, Visible, and Infrared Absorption Spectra of Single Crystal ThO_2

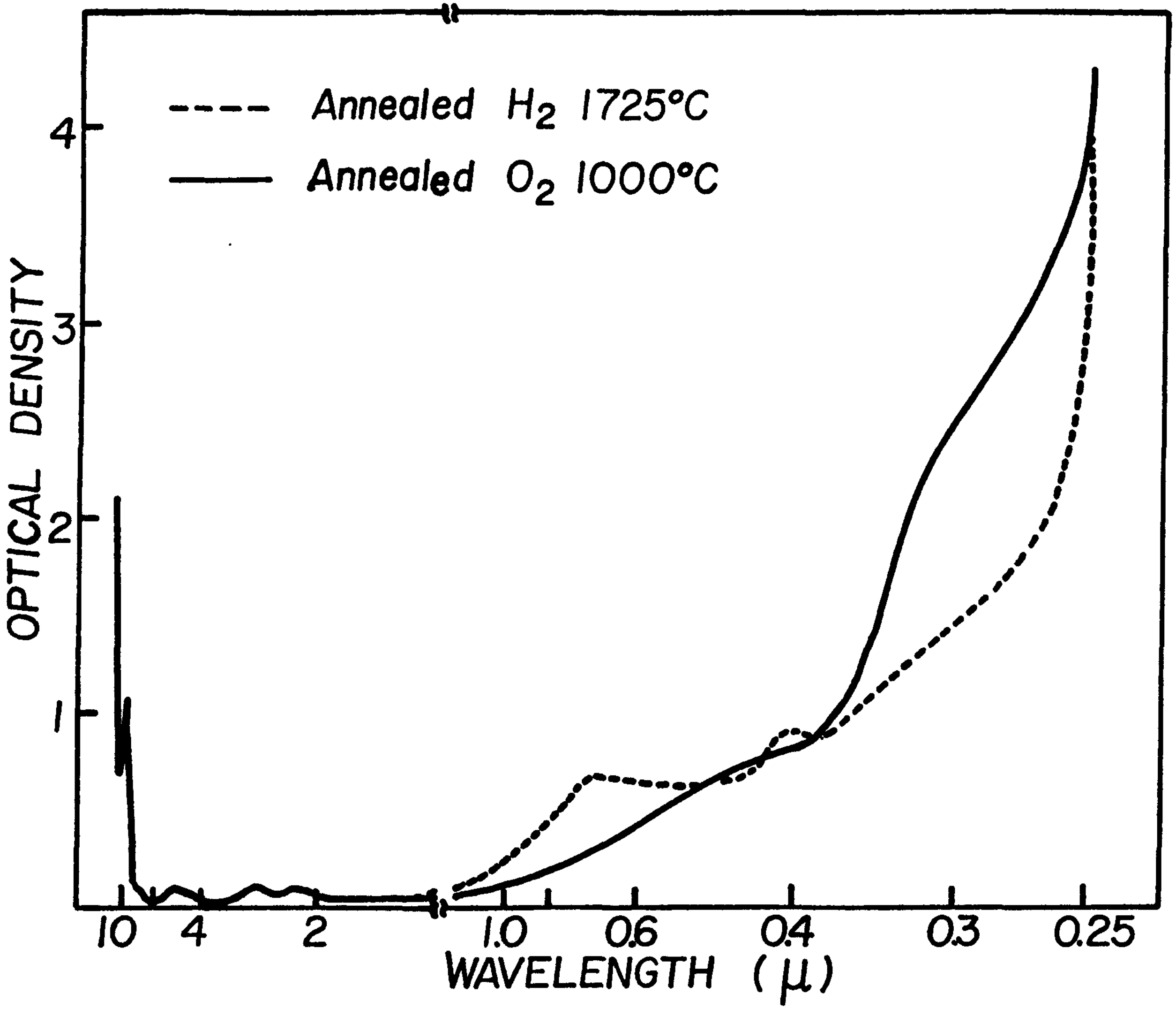


Fig. D.3 Ultraviolet, Visible, and Infrared Absorption Spectra of Single Crystal ThO_2

APPENDIX E

FORTRAN Program for the K-K Iterative Method

FORTRAN Implementation

Lorentz Oscillator:

Program Symbol	Definition
N	Number of segment
POL	Polarization
WI	Wavelength at short side (μ)
VO	Resonance wavelength (μ)
EO	Dielectric Constant at long wavelength
T	Strength of resonance
GARMA	Damping constant
THETA	Incidence angle (radian)
EPS	A positive number less than 10^{-5}
R	Reflectivity at normal incident angle
RO	Experimental reflectivity
ZN	Index of refraction
ZK	Extinction coefficient

Iterative K-K Analysis:

Program Symbol	Definition
M	Number of iteration
N	Number of Points
PHI	Incidence angle (radian)
POL	Polarization
RO(K)	Values of experimental reflectivity
THETA	Phase angle
X(K)	Wavelength (μ)

Index of Refraction from K-K Theory:

Program Symbol	Definition
E1	Dielectric constant at short wavelength (μ)
N	Number of Values
Y(K)	Values of wavelengths (μ)
ZN(K)	Values of index of refraction
ZK(K)	Values of extinction coefficient

APPENDIX F

FORTRAN Program for the Calculation of Surface Radiation Properties of ThO_2 and the Related Reactor Materials

FORTRAN Implementation

Spectral Hemispherical Properties:

Program Symbol	Definition
WA	Resonance wavelength
Y1	Index of refraction at medium 1
Y2	Index of refraction at medium 2
Z1	Extinction coefficient at medium 1
Z2	Extinction coefficient at medium 2

Total Hemispherical Properties:

Program Symbol	Definition
EO(I)	Values of spectral hemispherical emittance
TE	Source temperature
Y1(J)	Values of wavelength (μ)
VALUE	Total hemispherical emittance
VAL	Total hemispherical reflectance

```
@FOR, ASIZ
FOR RE7A-08/01/72-11:12:08

   MAIN PROGRAM

   STORAGE USED: CODE(1) 000224; DATA(0) 000115; BLANK COMMON(2) 000000


   EXTERNAL REFERENCES (BLOCK, NAME)

    0003   NINTR$
    0004   COS
    0005   SIN
    0006   TAN
    0007   SQRT
    0010   XPRR
    0011   NWDU$
    0012   NIO2$
    0013   NSTOP$


   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0000   000044 10F        0001   000054 110G       0001   000154 20L        0001   000165 30L        0001   000173 40L
    0001   000174 50L        0000 R 000026 AA         0000 R 000025 AAA        0000 R 000022 B          0000 R 000034 DS
    0000 R 000036 DO         0000 R 000023 ES         0000 R 000001 EPS        0000 R 000011 GAMMA      0000 I 000017 I
    0000 I 000000 N          0000 I 000012 NP1        0000 R 000037 P          0000 R 000007 PI         0000 R 000002 POL
    0000 R 000035 Q          0000 R 000075 QSQ        0000 R 000033 R          0000 R 000043 RO         0000 R 000042 R2
    0000 R 000041 RPS        0000 R 000021 SIV        0000 R 000024 SIVS       0000 R 000010 T          0000 R 000004 THETA
    0000 R 000015 V          0000 R 000016 VA         0000 R 000017 VB         0000 R 000005 VO         0000 R 000014 W
    0000 R 000003 WI         0000 R 000020 X          0000 R 000040 Z          0000 R 000032 ZK         0000 R 000031 ZKK
    0000 R 000030 ZN         0000 R 000027 ZNN


00101        1.           N=200                                                                       000000
00103        2.           EPS=0.0000001                                                               000003
00104        3.           POL=0.                                                                      000005
00105        4.           WI=0.                                                                       000006
00106        5.           THETA=1.0472                                                                000010
00107        6.           VO=10.0                                                                     000012
00110        7.           DS=0.7                                                                      000014
00111        8.           PI=3.141592                                                                 000016
00112        9.           T=0.063                                                                     000020
00113       10.           GAMMA=0.005                                                                 000022
00114       11.           NP1=N+1                                                                     000024
00115       12.           DO 1 I=1,NP1                                                                000054
00120       13.           W=WI+0.1*FLOAT(I-1)                                                         000064
00121       14.           V=VO/W                                                                      000074
00122       15.           VA=1.-V**2                                                                  000077
00123       16.           VB=GAMMA*V                                                                  000102
00124       17.           X=T*VA/(VA**2+VB**2)                                                        000105
00125       18.            SIV=2.*PI*T*VB/(VA**2+VB**2)                                               000114
00126       19.           R=RO+4.*PI*X                                                                000120
00127       20.           RS=R**2                                                                     000123
00130       21.           SIVS=SIV**2                                                                 000125
```

```
00131     22*            AAA=BS+4.*ST*S                                                                      000127
00132     23*            AA=SQRT(AAA)                                                                        000133
00133     24*            ZNN=0.5*(AA+B)                                                                      000136
00134     25*            ZNN=ABS(ZNN)                                                                        000141
00135     26*            IF(ZNN.LT.EPS)GO TO 20                                                              000143
00137     27*            ZN=SQRT(ZNN)                                                                        000146
00140     28*            GO TO 30                                                                            000152
00141     29*         20 ZN=0.                                                                               000154
00142     30*         30 ZKK=0.5*(AA-B)                                                                      000155
00143     31*            ZKK=ABS(ZKK)                                                                        000160
00144     32*            IF(ZKK.LT.EPS)GO TO 40                                                              000162
00145     33*            ZK=SQRT(ZKK)                                                                        000165
00147     34*            GO TO 50                                                                            000171
00150     35*         40 ZK=0.                                                                               000173
00151     36*         50 R=((ZN-1.)**2+ZK**2)/((ZN+1.)**2+ZK**2)                                             000174
00152     37*            BB=ZN**2-ZK**2-(SIN(THETA))**2                                                      000212
00153     38*            QSQ=(BB+(BB**2+4.*((ZN*ZK)**2))**.5)/2.                                             000221
00154     39*            Q=SQRT(QSQ)                                                                         000235
00155     40*            P=(ZN*ZK)/Q                                                                         000250
00156     41*            Z=((Q-COS(THETA))**2+P**2)/((Q+COS(THETA))**2+P**2)                                 000255
00157     42*            RPS=((Q-SIN(THETA)*TAN(THETA))**2+P**2)/((Q+SIN(THETA)*TAN(THETA)                   000264
00157     43*           *)**2+P**2)                                                                          000264
00160     44*            RP=RPS*Z                                                                            000272
00161     45*            RO=0.5*(Z*(1.+POL)+RP*(1.-POL))                                                     000274
00162     46*            WRITE(6,10)W,ZN,ZK,R,Z,RO                                                           000302
00172     47*         10 FORMAT(1H0,5X,'W= ',F10.5,5X,'ZN= ',F10.5,5X,'ZK= ',F10.5,5X,                       000317
00172     48*           $'R= ',F10.5,5X,'Z= ',F10.5,5X,'RO= ',F10.5)                                          000317
00173     49*          1 CONTINUE                                                                            000317
00175     50*            STOP                                                                                000317
00176     51*            END                                                                                 000323

     END OF COMPILATION:         NO  DIAGNOSTICS.
```

```
@FOR, ASIZ
FOR [illegible]/15/79-19:25:05

   MAIN PROGRAM

   STORAGE USED: CODE(1) 000600; DATA(0) 002753; BLANK COMMON(2) 000000


   EXTERNAL REFERENCES (BLOCK, NAME)

    0003   NINTR$
    0004   NRDU$
    0005   COS
    0006   SIN
    0007   TAN
    0010   NIO2$
    0011   NIO1$
    0012   NWDU$
    0013   ALOG
    0014   SQRT
    0015   XPRR
    0016   NSTOP$


   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0000   002621 10F        0001   000060 114C       0001   000065 120G       0001   000077 127C       0001   000104 133G
    0001   000112 141G       0001   000120 147G       0001   000125 155G       0001   000133 160G       0001   000174 171G
    0001   000200 175G       0001   000247 2L         0000   002624 20F        0001   000526 25L        0001   000446 253G
    0001   000470 26L        0001   000564 27L        0001   000504 276G       0001   000425 30L        0001   000542 321G
    0001   000572 37L        0001   000254 4L         0000   002626 40F        0001   000455 42L        0001   000466 44L
    0000   002630 50F        0001   000513 52L        0001   000524 54L        0001   000551 57L        0001   000562 59L
    0001   000441 70L        0001   000477 71L        0001   000535 74L        0000 R 000000 A          0000 R 002607 AMW
    0000 R 002610 APW        0000 R 000144 B          0000 R 000310 C          0000 R 000454 D          0000 I 002603 I
    0000 I 002620 II         0000 I 002577 ITER       0000 I 002605 J          0000 I 002575 JJ         0000 I 002574 K
    0000 I 002576 KK         0000 I 002600 L          0000 I 002601 LM1        0000 I 002570 M          0000 I 002571 N
    0000 I 002602 NM1        0000 R 000620 P          0000 R 002572 PHI        0000 R 002606 PI         0000 R 002614 PN
    0000 R 002573 POL        0000 R 002617 PQ         0000 R 002613 Q          0000 R 001604 R          0000 R 002612 RD
    0000 R 002114 RNEW       0000 R 002260 RO         0000 R 002615 RPS        0000 R 002616 RS         0000 R 002611 THESUP
    0000 R 001170 THETA      0000 R 002604 THETAA     0000 R 000764 U          0000 R 001750 W          0000 R 002424 X
    0000 R 001440 ZK         0000 R 001274 ZN


00101      1*          DIMENSION A(100),B(100),C(100),D(100),P(100),U(100),THETA(100),      000000
00101      2*         1ZN(100),ZK(100),R(100),W(100),RNEW(100),RO(100),X(100)               000000
00103      3*          READ(5,10)M,N,PHI,POL                                                000001
00111      4*       10 FORMAT(I3,I3,F10.4,F6.5)                                             000040
00112      5*          READ(5,20)(X(K),K=1,N),(RO(K),K=1,N)                                 000040
00124      6*       20 FORMAT(8F10.4)                                                       000070
00125      7*          WRITE(6,40)(X(K),K=1,N),(RO(K),K=1,N)                                000070
00137      8*       40 FORMAT(20X,5F10.4)                                                   000112
00140      9*          DO 111 JJ=1,N                                                        000112
00143     10*          W(JJ)=1000./X(JJ)                                                    000112
00144     11*      111 CONTINUE                                                             000120
00145     12*          DO 31 KK=1,N                                                         000120
```

```
00151     13*           R(KK)=RO(KK)                                                        000120
00152     14*        31 CONTINUE                                                            000125
00154     15*           DO 33 ITER=1,M                                                      000125
00157     16*           DO 80 L=2,N                                                         000133
00162     17*           LM1=L-1                                                             000133
00163     18*           A(L)=(1./2.)*(ALOG(R(L))-ALOG(R(LM1)))                              000137
00164     19*           B(L)=W(L)-W(LM1)                                                    000155
00165     20*        80 U(L)=A(L)/B(L)                                                      000160
00167     21*           NM1=N-1                                                             000164
00170     22*           DO 30 I=2,NM1                                                       000166
00173     23*           THETAA=0.                                                           000174
00174     24*           DO 4 J=2,NM1                                                        000200
00177     25*           P(J)=U(J+1)-U(J)                                                    000203
00200     26*           PI=3.141592                                                         000203
00201     27*           AMW=ABS(W(I)-W(J))                                                  000205
00202     28*           APW=ABS(W(I)+W(J))                                                  000211
00203     29*           D(J)=(W(I)+W(J))*(ALOG(APW))                                        000215
00204     30*           IF(I-J)3,2,3                                                        000224
00207     31*         3 C(J)=(W(I)-W(J))*(ALOG(AMW))                                        000227
00210     32*           THESUB=+(1./PI)*P(J)*(C(J)+D(J))                                    000237
00211     33*           GO TO 4                                                             000245
00212     34*         2 THESUB=+(1./PI)*P(J)*D(J)                                           000247
00213     35*         4 THETAA=THETAA+THESUB                                                000254
00215     36*           THETA(I)=THETAA                                                     000260
00216     37*           RD=1.+R(I)-2.*SQRT(R(I))*COS(THETA(I))                              000261
00217     38*           Q=(1.-R(I))*COS(PHI)/RD                                             000302
00220     39*           PN=2.*SQRT(R(I))*SIN(THETA(I))*COS(PHI)/RD                          000307
00221     40*           RPS=((Q-SIN(PHI)*TAN(PHI))**2+PN**2)/((Q+SIN(PHI)*TAN(PHI))**2+     000327
00221     41*          1PN**2)                                                              000327
00222     42*           RS=2.*RO(I)/((1.+POL)+RPS*(1.-POL))                                 000343
00223     43*           PQ=Q**2-PN**2+(SIN(PHI))**2                                         000351
00224     44*           ZN(I)=((PQ+(PQ**2+4.*(PN*Q)**2)**.5)/2.)**.5                        000356
00225     45*           ZK(I)=PN*Q/ZN(I)                                                    000402
00226     46*           RNEW(I)=RS                                                          000405
00227     47*           IF(ITER- 1 )30,61,61                                                000407
00232     48*        61 WRITE(6,53)ITER,X(I),RNEW(I),ZN(I),ZK(I)                            000412
00241     49*        53 FORMAT(5X,'M=',I3,10X,'X= ',F10.5,10X,'RNEW=',F10.5,10X,'ZN= ',     000427
00241     50*          $F10.5,10X,'ZK= ',F10.5)                                             000427
00242     51*        30 CONTINUE                                                            000427
00244     52*           IF(ITER- 7)70,71,72                                                 000427
00247     53*        72 IF(ITER-13)71,74,74                                                 000433
00252     54*        70 DO 26 II=2,NM1                                                      000441
00255     55*           IF(X(II)-10.09)41,41,42                                             000446
00260     56*        41 R(II)=RNEW(II)                                                      000451
00261     57*           GO TO 26                                                            000453
00262     58*        42 IF(X(II)-15.01)43,44,44                                             000455
00265     59*        43 R(II)=(RNEW(II)+R(II))/2.                                           000460
00266     60*           GO TO 26                                                            000464
00267     61*        44 R(II)=RNEW(II)                                                      000466
00270     62*        26 CONTINUE                                                            000471
00272     63*           R(1)=R(2)                                                           000471
00273     64*           R(N)=R(NM1)                                                         000473
00274     65*           GO TO 33                                                            000475
00275     66*        71 DO 25 II=2,NM1                                                      000477
00300     67*           IF(X(II)-10.19)51,51,52                                             000504
00303     68*        51 R(II)=RNEW(II)                                                      000507
00304     69*           GO TO 25                                                            000511
```

```
00305     70*          52 IF(X(II)-13.01)53,54,54                                        000513
00310     71*          53 R(II)=(RNEW(II)+R(II))/2.                                      000516
00311     72*             GO TO 25                                                       000522
00312     73*          54 R(II)=RNEW(II)                                                 000524
00313     74*          25 CONTINUE                                                       000527
00315     75*             R(1)=R(2)                                                      000527
00316     76*             R(N)=R(NM1)                                                    000531
00317     77*             GO TO 33                                                       000533
00320     78*          24 DO 27 II=2,NM1                                                 000535
00323     79*             IF(X(II)-13.29)56,56,57                                        000542
00326     80*          56 R(II)=RNEW(II)                                                 000545
00327     81*             GO TO 27                                                       000547
00330     82*          57 IF(X(II)-13.51)58,59,59                                        000551
00333     83*          58 R(II)=(RNEW(II)+R(II))/2.                                      000554
00334     84*             GO TO 27                                                       000560
00335     85*          59 R(II)=RNEW(II)                                                 000562
00336     86*          27 CONTINUE                                                       000565
00340     87*             R(1)=R(2)                                                      000565
00341     88*             R(N)=R(NM1)                                                    000567
00342     89*          33 CONTINUE                                                       000573
00344     90*             STOP                                                           000573
00345     91*             END                                                            000577

     END OF COMPILATION:       NO  DIAGNOSTICS.
```

```
       2.0000     2.2000     3.0000     3.5000     4.0000     4.5000     5.0000     5.5000
       6.0000     7.0000     7.5000     8.0000     8.2000     8.4000     8.6000     8.8000
       9.0000     9.2000     9.4000     9.6000     9.8000     9.9000    10.0000    10.1000
      10.2000    10.3000    10.4000    10.5000    10.6000    10.7000    10.8000    11.0000
      11.2000    11.4000    11.6000    12.0000    12.2000    12.4000    12.5000    12.6000
      12.7000    12.8000    12.9000    13.0000    13.1000    13.2000    13.3000    13.4000
      13.5000    13.6000    13.8000    14.0000    14.5000    15.0000    15.5000    16.0000
      16.5000    17.0000    17.5000    18.0000      .2282      .2262      .2259      .2242
        .2222      .2197      .2167      .2131      .2087      .1963      .1874      .1757
        .1698      .1632      .1554      .1463      .1353      .1219      .1049      .0823
        .0499      .0279      .0749      .1694      .7104      .8369      .8858      .9120
        .9278      .9364      .9459      .9556      .9613      .9647      .9666      .9659
        .9623      .9517      .9368      .8631      .7225      .6471      .5984      .5631
        .5358      .5138      .4956      .4803      .4671      .4556      .4366      .4214
        .3896      .3754      .3621      .3525      .3442      .3378      .3283      .3283
M=  1        X=   2.20000         RNEW=    .45595          ZN=   1.65797          ZK=     -.02534
M=  1        X=   3.00000         RNEW=    .45124          ZN=   1.65001          ZK=     -.03255
M=  1        X=   3.50000         RNEW=    .44774          ZN=   1.64409          ZK=     -.03778
M=  1        X=   4.00000         RNEW=    .44361          ZN=   1.63710          ZK=     -.04352
M=  1        X=   4.50000         RNEW=    .43945          ZN=   1.62845          ZK=     -.04926
M=  1        X=   5.00000         RNEW=    .43225          ZN=   1.61910          ZK=     -.05556
M=  1        X=   5.50000         RNEW=    .42479          ZN=   1.60576          ZK=     -.06211
M=  1        X=   6.00000         RNEW=    .41566          ZN=   1.59796          ZK=     -.06311
M=  1        X=   7.00000         RNEW=    .38974          ZN=   1.54884          ZK=     -.08710
M=  1        X=   7.50000         RNEW=    .37111          ZN=   1.51989          ZK=     -.09478
M=  1        X=   8.00000         RNEW=    .34651          ZN=   1.48209          ZK=     -.10473
M=  1        X=   8.20000         RNEW=    .33412          ZN=   1.46379          ZK=     -.10749
M=  1        X=   8.40000         RNEW=    .32024          ZN=   1.44341          ZK=     -.11061
M=  1        X=   8.60000         RNEW=    .30385          ZN=   1.41979          ZK=     -.11335
M=  1        X=   8.80000         RNEW=    .28476          ZN=   1.39279          ZK=     -.11556
M=  1        X=   9.00000         RNEW=    .26175          ZN=   1.36102          ZK=     -.11675
M=  1        X=   9.20000         RNEW=    .23367          ZN=   1.32354          ZK=     -.11627
M=  1        X=   9.40000         RNEW=    .19885          ZN=   1.27309          ZK=     -.11252
M=  1        X=   9.60000         RNEW=    .15311          ZN=   1.22107          ZK=     -.10266
M=  1        X=   9.80000         RNEW=    .08950          ZN=   1.13987          ZK=     -.08597
M=  1        X=   9.90000         RNEW=    .04849          ZN=   1.08882          ZK=     -.06382
M=  1        X=  10.00000         RNEW=    .00781          ZN=    .99576          ZK=     -.03464
M=  1        X=  10.10000         RNEW=    .22068          ZN=    .88369          ZK=     -.04380
M=  1        X=  10.20000         RNEW=    .77035          ZN=    .78213          ZK=     -.03272
M=  1        X=  10.30000         RNEW=    .88885          ZN=    .62567          ZK=     -.05321
M=  1        X=  10.40000         RNEW=    .93766          ZN=    .40985          ZK=     -.09640
M=  1        X=  10.50000         RNEW=    .95662          ZN=    .13896          ZK=     -.33410
M=  1        X=  10.60000         RNEW=    .97029          ZN=    .08877          ZK=     -.61557
M=  1        X=  10.70000         RNEW=    .97938          ZN=    .07750          ZK=     -.83087
M=  1        X=  10.80000         RNEW=    .98581          ZN=    .07453          ZK=    -1.02300
M=  1        X=  11.00000         RNEW=    .99430          ZN=    .07844          ZK=    -1.38934
M=  1        X=  11.20000         RNEW=    .99974          ZN=    .09138          ZK=    -1.77736
M=  1        X=  11.40000         RNEW=   1.00367          ZN=    .11525          ZK=    -2.22944
M=  1        X=  11.60000         RNEW=   1.00681          ZN=    .15819          ZK=    -2.80717
M=  1        X=  12.00000         RNEW=   1.01257          ZN=    .45779          ZK=    -4.98073
M=  1        X=  12.20000         RNEW=   1.01616          ZN=   1.29569          ZK=    -8.02623
M=  1        X=  12.40000         RNEW=   1.02213          ZN=  15.50962          ZK=   -19.63038
M=  1        X=  12.50000         RNEW=   1.02945          ZN=  16.06409          ZK=    15.07663
M=  1        X=  12.60000         RNEW=   1.04752          ZN=   4.66971          ZK=     6.39406
M=  1        X=  12.70000         RNEW=   1.04350          ZN=   3.65975          ZK=     2.97209
M=  1        X=  12.80000         RNEW=   1.01577          ZN=   3.42097          ZK=     1.99679
M=  1        X=  12.90000         RNEW=    .98719          ZN=   3.23372          ZK=     1.56092
```

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M=  1        X=  13.00000       RNEW=   .96062       ZN=   3.08307       ZK=   1.19783
M=  1        X=  13.10000       RNEW=   .93652       ZN=   2.96100       ZK=    .99258
M=  1        X=  13.20000       RNEW=   .91480       ZN=   2.86067       ZK=    .84403
M=  1        X=  13.30000       RNEW=   .89526       ZN=   2.77707       ZK=    .73147
M=  1        X=  13.40000       RNEW=   .87772       ZN=   2.70669       ZK=    .64368
M=  1        X=  13.50000       RNEW=   .86176       ZN=   2.64567       ZK=    .57301
M=  1        X=  13.60000       RNEW=   .84726       ZN=   2.59335       ZK=    .51428
M=  1        X=  13.80000       RNEW=   .82199       ZN=   2.50577       ZK=    .42667
M=  1        X=  14.00000       RNEW=   .80065       ZN=   2.43612       ZK=    .36319
M=  1        X=  14.50000       RNEW=   .75295       ZN=   2.29469       ZK=    .24103
M=  1        X=  15.00000       RNEW=   .73056       ZN=   2.22730       ZK=    .17175
M=  1        X=  15.50000       RNEW=   .70858       ZN=   2.17876       ZK=    .13130
M=  1        X=  16.00000       RNEW=   .69147       ZN=   2.13551       ZK=    .09787
M=  1        X=  16.50000       RNEW=   .67800       ZN=   2.10245       ZK=    .07094
M=  1        X=  17.00000       RNEW=   .66677       ZN=   2.07541       ZK=    .04795
M=  1        X=  17.90000       RNEW=   .64960       ZN=   2.03521       ZK=    .00423
M=  2        X=   2.20000       RNEW=   .42654       ZN=   2.72067       ZK=   -.01172
M=  2        X=   3.00000       RNEW=   .42348       ZN=   2.68958       ZK=   -.00627
M=  2        X=   3.50000       RNEW=   .42119       ZN=   2.66686       ZK=   -.00418
M=  2        X=   4.00000       RNEW=   .41847       ZN=   2.64044       ZK=   -.00305
M=  2        X=   4.50000       RNEW=   .41501       ZN=   2.60794       ZK=   -.00134
M=  2        X=   5.00000       RNEW=   .41080       ZN=   2.56965       ZK=   -.00047
M=  2        X=   5.50000       RNEW=   .40564       ZN=   2.52472       ZK=    .00119
M=  2        X=   6.00000       RNEW=   .39919       ZN=   2.47133       ZK=    .00653
M=  2        X=   7.00000       RNEW=   .38319       ZN=   2.32862       ZK=   -.00618
M=  2        X=   7.50000       RNEW=   .36579       ZN=   2.23348       ZK=   -.00430
M=  2        X=   8.00000       RNEW=   .34594       ZN=   2.11622       ZK=   -.01140
M=  2        X=   8.20000       RNEW=   .33556       ZN=   2.06056       ZK=   -.01116
M=  2        X=   8.40000       RNEW=   .32366       ZN=   2.00062       ZK=   -.01278
M=  2        X=   8.60000       RNEW=   .30925       ZN=   1.93296       ZK=   -.01513
M=  2        X=   8.80000       RNEW=   .29198       ZN=   1.85806       ZK=   -.01810
M=  2        X=   9.00000       RNEW=   .27952       ZN=   1.77295       ZK=   -.02181
M=  2        X=   9.20000       RNEW=   .24366       ZN=   1.67664       ZK=   -.02601
M=  2        X=   9.40000       RNEW=   .20874       ZN=   1.56497       ZK=   -.02972
M=  2        X=   9.60000       RNEW=   .16158       ZN=   1.43233       ZK=   -.03164
M=  2        X=   9.80000       RNEW=   .09435       ZN=   1.26367       ZK=   -.04439
M=  2        X=   9.90000       RNEW=   .05065       ZN=   1.16212       ZK=   -.03614
M=  2        X=  10.00000       RNEW=   .00796       ZN=   1.01134       ZK=   -.04532
M=  2        X=  10.10000       RNEW=   .22479       ZN=    .86704       ZK=   -.07838
M=  2        X=  10.20000       RNEW=   .77614       ZN=    .70281       ZK=   -.05701
M=  2        X=  10.30000       RNEW=   .89191       ZN=    .39927       ZK=   -.12495
M=  2        X=  10.40000       RNEW=   .93327       ZN=    .11936       ZK=   -.47189
M=  2        X=  10.50000       RNEW=   .95312       ZN=    .08121       ZK=   -.76726
M=  2        X=  10.60000       RNEW=   .96408       ZN=    .06891       ZK=   -.99384
M=  2        X=  10.70000       RNEW=   .97075       ZN=    .06279       ZK=  -1.19145
M=  2        X=  10.80000       RNEW=   .97503       ZN=    .05934       ZK=  -1.37461
M=  2        X=  11.00000       RNEW=   .97977       ZN=    .05627       ZK=  -1.72079
M=  2        X=  11.20000       RNEW=   .98167       ZN=    .05624       ZK=  -2.06676
M=  2        X=  11.40000       RNEW=   .98260       ZN=    .05857       ZK=  -2.43292
M=  2        X=  11.60000       RNEW=   .98250       ZN=    .06753       ZK=  -2.94240
M=  2        X=  12.00000       RNEW=   .97989       ZN=    .09161       ZK=  -3.94066
M=  2        X=  12.20000       RNEW=   .97674       ZN=    .13365       ZK=  -4.82477
M=  2        X=  12.40000       RNEW=   .96965       ZN=    .27975       ZK=  -6.40517
M=  2        X=  12.50000       RNEW=   .96045       ZN=    .60290       ZK=  -8.09271
M=  2        X=  12.60000       RNEW=   .92141       ZN=   3.06891       ZK= -11.11707
M=  2        X=  12.70000       RNEW=   .85559       ZN=   8.74957       ZK=  -7.96124
M=  2        X=  12.80000       RNEW=   .82199       ZN=   8.48655       ZK=  -4.46860
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M= 39          X=    4.50000          RNEW=    .41941          ZN=    2.49268          ZK=    -.02693
M= 39          X=    5.00000          RNEW=    .41469          ZN=    2.46538          ZK=    -.02878
M= 39          X=    5.50000          RNEW=    .40898          ZN=    2.43291          ZK=    -.02994
M= 39          X=    6.00000          RNEW=    .40193          ZN=    2.39376          ZK=    -.02764
M= 39          X=    7.00000          RNEW=    .38152          ZN=    2.28507          ZK=    -.03891
M= 39          X=    7.50000          RNEW=    .36642          ZN=    2.20965          ZK=    -.03600
M= 39          X=    8.00000          RNEW=    .34597          ZN=    2.11289          ZK=    -.03839
M= 39          X=    8.20000          RNEW=    .33541          ZN=    2.06548          ZK=    -.03574
M= 39          X=    8.40000          RNEW=    .32339          ZN=    2.01330          ZK=    -.03412
M= 39          X=    8.60000          RNEW=    .30893          ZN=    1.95297          ZK=    -.03246
M= 39          X=    8.80000          RNEW=    .29169          ZN=    1.88427          ZK=    -.03056
M= 39          X=    9.00000          RNEW=    .27038          ZN=    1.80388          ZK=    -.02872
M= 39          X=    9.20000          RNEW=    .24376          ZN=    1.70988          ZK=    -.02677
M= 39          X=    9.40000          RNEW=    .20913          ZN=    1.59704          ZK=    -.02447
M= 39          X=    9.60000          RNEW=    .16216          ZN=    1.45829          ZK=    -.02204
M= 39          X=    9.80000          RNEW=    .09480          ZN=    1.27858          ZK=    -.03650
M= 39          X=    9.90000          RNEW=    .05083          ZN=    1.16944          ZK=    -.03089
M= 39          X=   10.00000          RNEW=    .00796          ZN=    1.01199          ZK=    -.04573
M= 39          X=   10.10000          RNEW=    .22203          ZN=     .86037          ZK=    -.07995
M= 39          X=   10.20000          RNEW=    .77031          ZN=     .67862          ZK=    -.05773
M= 39          X=   10.30000          RNEW=    .88476          ZN=     .31118          ZK=    -.15100
M= 39          X=   10.40000          RNEW=    .92634          ZN=     .09151          ZK=    -.57525
M= 39          X=   10.50000          RNEW=    .94668          ZN=     .06754          ZK=    -.86850
M= 39          X=   10.60000          RNEW=    .95868          ZN=     .05948          ZK=   -1.10378
M= 39          X=   10.70000          RNEW=    .96627          ZN=     .05605          ZK=   -1.31424
M= 39          X=   10.80000          RNEW=    .97146          ZN=     .05489          ZK=   -1.51300
M= 39          X=   11.00000          RNEW=    .97792          ZN=     .05651          ZK=   -1.89808
M= 39          X=   11.20000          RNEW=    .98160          ZN=     .06220          ZK=   -2.29439
M= 39          X=   11.40000          RNEW=    .98380          ZN=     .07229          ZK=   -2.72666
M= 39          X=   11.60000          RNEW=    .98511          ZN=     .08865          ZK=   -3.22607
M= 39          X=   12.00000          RNEW=    .98543          ZN=     .16894          ZK=   -4.64876
M= 39          X=   12.20000          RNEW=    .98415          ZN=     .28838          ZK=   -5.86438
M= 39          X=   12.40000          RNEW=    .97989          ZN=     .71742          ZK=   -8.29220
M= 39          X=   12.50000          RNEW=    .97335          ZN=    1.74080          ZK=  -11.15841
M= 39          X=   12.60000          RNEW=    .94111          ZN=    8.59705          ZK=  -14.43840
M= 39          X=   12.70000          RNEW=    .87067          ZN=   12.19541          ZK=   -5.24964
M= 39          X=   12.80000          RNEW=    .82721          ZN=    9.86012          ZK=   -2.65879
M= 39          X=   12.90000          RNEW=    .79646          ZN=    8.46125          ZK=   -1.77450
M= 39          X=   13.00000          RNEW=    .77263          ZN=    7.56868          ZK=   -1.34203
M= 39          X=   13.10000          RNEW=    .75320          ZN=    6.94576          ZK=   -1.08846
M= 39          X=   13.20000          RNEW=    .73684          ZN=    6.48278          ZK=    -.92332
M= 39          X=   13.30000          RNEW=    .72279          ZN=    6.12374          ZK=    -.80900
M= 39          X=   13.40000          RNEW=    .71059          ZN=    5.83784          ZK=    -.72490
M= 39          X=   13.50000          RNEW=    .69977          ZN=    5.60214          ZK=    -.65998
M= 39          X=   13.60000          RNEW=    .69010          ZN=    5.40407          ZK=    -.61061
M= 39          X=   13.80000          RNEW=    .67362          ZN=    5.09353          ZK=    -.53087
M= 39          X=   14.00000          RNEW=    .65994          ZN=    4.85817          ZK=    -.47129
M= 39          X=   14.50000          RNEW=    .62977          ZN=    4.36937          ZK=    -.40695
M= 39          X=   15.00000          RNEW=    .61553          ZN=    4.18899          ZK=    -.40439
M= 39          X=   15.50000          RNEW=    .60178          ZN=    4.01561          ZK=    -.37028
M= 39          X=   16.00000          RNEW=    .59102          ZN=    3.88530          ZK=    -.35887
M= 39          X=   16.50000          RNEW=    .58251          ZN=    3.78589          ZK=    -.35599
M= 39          X=   17.00000          RNEW=    .57539          ZN=    3.70469          ZK=    -.35878
M= 39          X=   17.90000          RNEW=    .56455          ZN=    3.57793          ZK=    -.39656
M= 40          X=    2.20000          RNEW=    .43253          ZN=    2.57114          ZK=    -.02108
M= 40          X=    3.00000          RNEW=    .42901          ZN=    2.54977          ZK=    -.02197
M= 40          X=    3.50000          RNEW=    .42639          ZN=    2.53403          ZK=    -.02352
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M= 40      X=   4.00000      RNEW=   .42330      ZN=   2.51558      ZK=    -.02545
M= 40      X=   4.50000      RNEW=   .41941      ZN=   2.49268      ZK=    -.02697
M= 40      X=   5.00000      RNEW=   .41469      ZN=   2.46538      ZK=    -.02886
M= 40      X=   5.50000      RNEW=   .40898      ZN=   2.43292      ZK=    -.02982
M= 40      X=   6.00000      RNEW=   .40193      ZN=   2.39376      ZK=    -.02784
M= 40      X=   7.00000      RNEW=   .38152      ZN=   2.28507      ZK=    -.03987
M= 40      X=   7.50000      RNEW=   .36642      ZN=   2.20965      ZK=    -.03604
M= 40      X=   8.00000      RNEW=   .34597      ZN=   2.11269      ZK=    -.03840
M= 40      X=   8.20000      RNEW=   .33541      ZN=   2.06548      ZK=    -.03567
M= 40      X=   8.40000      RNEW=   .32339      ZN=   2.01330      ZK=    -.03411
M= 40      X=   8.60000      RNEW=   .30893      ZN=   1.95293      ZK=    -.03247
M= 40      X=   8.80000      RNEW=   .29169      ZN=   1.88427      ZK=    -.03059
M= 40      X=   9.00000      RNEW=   .27038      ZN=   1.80365      ZK=    -.02873
M= 40      X=   9.20000      RNEW=   .24376      ZN=   1.70988      ZK=    -.02676
M= 40      X=   9.40000      RNEW=   .20913      ZN=   1.59704      ZK=    -.02447
M= 40      X=   9.60000      RNEW=   .16216      ZN=   1.45829      ZK=    -.02203
M= 40      X=   9.80000      RNEW=   .09480      ZN=   1.27858      ZK=    -.03650
M= 40      X=   9.90000      RNEW=   .05083      ZN=   1.16945      ZK=    -.03089
M= 40      X=  10.00000      RNEW=   .00796      ZN=   1.01199      ZK=    -.04573
M= 40      X=  10.10000      RNEW=   .22202      ZN=    .86037      ZK=    -.07994
M= 40      X=  10.20000      RNEW=   .77031      ZN=    .67862      ZK=    -.05773
M= 40      X=  10.30000      RNEW=   .88476      ZN=    .31120      ZK=    -.15099
M= 40      X=  10.40000      RNEW=   .92634      ZN=    .09151      ZK=    -.57523
M= 40      X=  10.50000      RNEW=   .94688      ZN=    .06754      ZK=    -.86848
M= 40      X=  10.60000      RNEW=   .95868      ZN=    .05948      ZK=   -1.10350
M= 40      X=  10.70000      RNEW=   .96627      ZN=    .05605      ZK=   -1.31426
M= 40      X=  10.80000      RNEW=   .97145      ZN=    .05489      ZK=   -1.51295
M= 40      X=  11.00000      RNEW=   .97792      ZN=    .05651      ZK=   -1.89807
M= 40      X=  11.20000      RNEW=   .98160      ZN=    .06220      ZK=   -2.29434
M= 40      X=  11.40000      RNEW=   .98380      ZN=    .07229      ZK=   -2.72672
M= 40      X=  11.60000      RNEW=   .98511      ZN=    .08865      ZK=   -3.22610
M= 40      X=  12.00000      RNEW=   .98543      ZN=    .16893      ZK=   -4.64866
M= 40      X=  12.20000      RNEW=   .98415      ZN=    .28835      ZK=   -5.88399
M= 40      X=  12.40000      RNEW=   .97989      ZN=    .71735      ZK=   -8.29175
M= 40      X=  12.50000      RNEW=   .97335      ZN=   1.74071      ZK=  -11.15813
M= 40      X=  12.60000      RNEW=   .94111      ZN=   8.59324      ZK=  -14.43625
M= 40      X=  12.70000      RNEW=   .87067      ZN=  12.19351      ZK=   -5.25138
M= 40      X=  12.80000      RNEW=   .82721      ZN=   9.85938      ZK=   -2.66004
M= 40      X=  12.90000      RNEW=   .79646      ZN=   8.46114      ZK=   -1.77478
M= 40      X=  13.00000      RNEW=   .77263      ZN=   7.56850      ZK=   -1.34254
M= 40      X=  13.10000      RNEW=   .75320      ZN=   6.94561      ZK=   -1.08887
M= 40      X=  13.20000      RNEW=   .73684      ZN=   6.48271      ZK=    -.92357
M= 40      X=  13.30000      RNEW=   .72279      ZN=   6.12367      ZK=    -.80922
M= 40      X=  13.40000      RNEW=   .71059      ZN=   5.83784      ZK=    -.72496
M= 40      X=  13.50000      RNEW=   .69977      ZN=   5.60214      ZK=    -.65999
M= 40      X=  13.60000      RNEW=   .69010      ZN=   5.40403      ZK=    -.61082
M= 40      X=  13.80000      RNEW=   .67362      ZN=   5.09355      ZK=    -.53079
M= 40      X=  14.00000      RNEW=   .65994      ZN=   4.85819      ZK=    -.47114
M= 40      X=  14.50000      RNEW=   .62977      ZN=   4.38935      ZK=    -.40701
M= 40      X=  15.00000      RNEW=   .61553      ZN=   4.16900      ZK=    -.40432
M= 40      X=  15.50000      RNEW=   .60178      ZN=   4.01559      ZK=    -.37035
M= 40      X=  16.00000      RNEW=   .59102      ZN=   3.86528      ZK=    -.35896
M= 40      X=  16.50000      RNEW=   .58251      ZN=   3.78587      ZK=    -.35607
M= 40      X=  17.00000      RNEW=   .57539      ZN=   3.70466      ZK=    -.35891
M= 40      X=  17.90000      RNEW=   .56455      ZN=   3.57791      ZK=    -.39659
&FIN
```

```
@FOR, ASIS
FOR [illegible]

   MAIN PROGRAM

   STORAGE USED: CODE(1) [illegible]; DATA(0) [illegible]; BLANK COMMON(2) 000000

   EXTERNAL REFERENCES (BLOCK, NAME)

    0003   NINTR$
    0004   NRDU$
    0005   NIO2$
    0006   NIO1$
    0007   NWDU$
    0010   [illegible]
    0011   ALOG
    0012   NSTOP$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0000   004250 10L       0001   000025 1010      0001 L 000030 115G    0001   000044 1740      0001   000061 1750
    0001   000053 1700      0001   000100 1400      0001   000111 150L    0001   000133 1650      0001   000137 1710
    0001   000000 2L        0000   004251 [illegible] 0001   000030 4L  0000   004253 INJP$     0000   004256 EDF
    0000 R 000000 A         0000 R 004244 AMW       0000 R 004245 APL     0000 R 000310 B       0000 R 000000 C
    0000 R 001130 D         0000 R 004247 C1        0000 I 004240 T       0000 I 004235 II      0000 I 004242 J
    0000 I 004233 JJ        0000 I 004231 K         0000 I 004236 L       0000 I 004237 LM1     0000 I 004230 N
    0000 I 004234 NM1       0000 R 004440 F         0000 R 004243 PT      0000 R 003410 R       0000 R 001750 U
    0000 R 001620 W         0000 R 004... X         0000 R 000620 Y       0000 R 003100 ZK      0000 R 002570 ZN
    0000 R 004241 ZKK       0000 R 004246 ZC


00101      1*            DIMENSION A(200),B(200),C(200),D(200),P(200),U(200),W(200),                000000
00101      2*           1ZN(200),ZK(200),R(200),Y(200)                                               000000
00103      3*            READ(5,10)N                                                                  000001
00106      4*         10 FORMAT(I3)                                                                   000007
00107      5*            READ(5,20)(Y(K),K=1,N),(ZK(K),K=1,N)                                         000007
00121      6*         20 FORMAT(8F10.5)                                                               000035
00122      7*            WRITE(6,40)(Y(K),K=1,N),(ZK(K),K=1,N)                                        000035
00134      8*         40 FORMAT(20X,8(F10.6,2X))                                                      000054
00135      9*            X=0.7                                                                        000054
00136     10*            DO 30 JJ=1,N                                                                 000056
00141     11*         30 W(JJ)=1000./Y(JJ)                                                            000065
00143     12*            NM1=N-1                                                                      000070
00144     13*            DO 33 II=2,NM1                                                               000072
00147     14*            R(II)=ZK(II)                                                                 000100
00151     15*         33 CONTINUE                                                                     000102
00153     16*            R(1)=R(2)                                                                    000102
00154     17*            R(N)=R(NM1)                                                                  000104
00155     18*            DO 50 L=2,N                                                                  000111
00157     19*            LM1=L-1                                                                      000111
00161     20*            A(L)=R(L)-R(LM1)                                                             000115
00162     21*            B(L)=W(L)-W(LM1)                                                             000120
00163     22*          5 D(L)=A(L)/B(L)                                                               000123
```

```
00171     23*           DO 10 I=2,NM1                                                        000133
00167     24*           ZNN=0.                                                               000133
00170     25*           DO 4 J=2,NM1                                                         000137
00173     26*           B(J)=U(J+1)-U(J)                                                     000137
00174     27*           PI=3.141593                                                          000142
00175     28*           AMW=ABS(W(I)-W(J))                                                   000144
00176     29*           APW=ABS(W(I)+W(J))                                                   000150
00177     30*           D(J)=(W(I)+W(J))*(ALOG(APW))                                         000154
00200     31*           IF(I-J) 3,2,3                                                        000163
00203     32*         3 C(J)=(W(J)-W(I))*(ALOG(AMW))                                         000166
00204     33*           ZZN=-(1./PI)*B(J)*(C(J)+D(J))                                        000176
00205     34*           GO TO 4                                                              000204
00206     35*         2 ZZN=-(1./PI)*B(J)*(D(J))                                             000206
00207     36*         4 ZNN=ZNN+ZZN                                                          000213
00211     37*           ZN(I)=ZNN                                                            000217
00212     38*           ZI=SQRT(X)                                                           000220
00213     39*           ZN(I)=ZN(I)+ZI                                                       000222
00214     40*           WRITE(6,50)Y(I),ZN(I),ZK(I)                                          000224
00221     41*        50 FORMAT(20X,'Y(I)= ',F10.7,10X,'ZN(I)= ',F10.7,10X,'ZK(I)= ',F10.7)   000236
00222     42*        10 CONTINUE                                                             000236
00224     43*           STOP                                                                 000235
00225     44*           END                                                                  000242

      END OF COMPILATION:        NO  DIAGNOSTICS.
```

```
@MAP, IS
MAP [illegible]-A [illegible] [illegible]
ADDRESS LIMITS  [illegible]  [illegible]  [illegible] DECIMAL
                [illegible]  [illegible]  [illegible] DECIMAL
STARTING ADDRESS [illegible]

          SEGMENT MAIN          [illegible]       [illegible]

NSVTC$/FOR[illegible]        $(1)   [illegible] [illegible]                                 05 APR 73   20:07:01
NRDLK$/FOR-[illegible]       $(1)   001025 [illegible]047                                   25 APR 74   17:40:27
NINT[illegible]$/FOR-[illegible] $(1) [illegible]                $(2)   [illegible]         27 JUN 75   10:05:24
NW[illegible]$/FOR-[illegible]   $(1) [illegible]                $(2)   [illegible]         29 APR 74   17:49:58
NRWND$/FOR-[illegible]       $(1)   [illegible] [illegible]1414  $(2)   [illegible]         27 JUN 75   10:07:02
NCL[illegible]S$/FOR-[illegible] $(1) [illegible]                $(2)   [illegible]         16 APR 75   17:14:09
[illegible]$/FOR[illegible]  $(1)   [illegible] [illegible]      $(2)   [illegible]         12 MAY 71   15:54:25
N[illegible]H$/FOR-[illegible] $(1) [illegible]                  $(2)   [illegible]         29 APR 74   17:47:54
NI[illegible]$/FOR-[illegible] $(1) [illegible]                  $(2)   [illegible]         16 APR 75   17:24:12
NINTN[illegible]$/FOR-[illegible] $(1) [illegible]               $(2)   [illegible]         01 MAY 73   09:10:58
NI[illegible]$/FOR-[illegible] $(1) [illegible]                  $(2)   [illegible]         29 APR 74   17:47:56
NOTIN$/FOR-[illegible]       $(1)   [illegible]                  $(2)   [illegible]         16 APR 75   17:2[illegible]:59
NB[illegible]L$/FOR-[illegible] $(1) [illegible]                                            16 APR 75   17:13:54
NDF[illegible]$                                                  $(2)   [illegible]         23 JUN 75   09:[illegible]:12
NU[illegible]A$/FOR[illegible] $(1) [illegible]                                             10 JUL 72   21:41:26
NTA[illegible]$/FOR-[illegible]                                  $(2)   [illegible]         11 MAR 75   15:[illegible]:08
NWBLK$/FOR[illegible]        $(1)   [illegible]                                             10 JUL 72   21:41:28
NFCHK$/FOR-[illegible]       $(1)   [illegible]                  $(2)   [illegible]         27 JUN 75   10:05:10
                             $(7)   [illegible]                  $(4)   [illegible]
FOR[illegible]/FOR[illegible]                                    $(2)   [illegible]         11 MAR 75   10:0[illegible]:49
NCNV[illegible]/FOR[illegible] $(1) [illegible]                  $(2)   [illegible]         10 JUL 72   21:40:13
NFTV[illegible]/FOR-[illegible] $(1) [illegible]                                            29 APR 74   17:47:54
NFM[illegible]$/FOR-[illegible] $(1) [illegible]                 $(2)   [illegible]         16 APR 75   17:20:52
NB[illegible]/FOR-[illegible] $(1)  [illegible]                  $(2)   [illegible]         16 APR 75   17:17:46
NOUT$/FOR-[illegible]        $(1)   [illegible] 010556           $(2)   043134 [illegible]  01 MAY 73   09:1[illegible]:49
NIOER$/FOR-[illegible]       $(1)   [illegible]                  $(2)   043176 [illegible]  23 JUN 75   10:05:47
NOCU[illegible]/FOR[illegible] $(1) [illegible]                                             10 JUL 72   21:41:08
NE[illegible]/FOR-[illegible] $(1)  [illegible]                  $(2)   [illegible]         11 MAR 75   15:[illegible]:59
ERU$/SYS[illegible]                                                                         10 JAN 73   15:23:45
NE[illegible]$/FOR-[illegible] $(1) [illegible]                  $(2)   [illegible]         27 JUN 75   10:01:29
ALOC$/FOR-[illegible]        $(1)   [illegible]                  $(2)   [illegible]         17 APR 75   09:40:35
N[illegible]$/FOR-[illegible] $(1)  [illegible]                  $(2)   [illegible]         16 APR 75   17:27:49
FORVCOM$/FOR-[illegible]                                         $(2)   [illegible]         11 MAR 75   15:[illegible]:31
N[illegible]/FOR-[illegible] $(1)   [illegible]                  $(2)   [illegible]         11 MAR 75   15:34:50
BLANK$COMMON(COMMON BLOCK)
NAM[illegible]               $(1)   [illegible]                  $(0)   043747 [illegible]  21 APR 73   15:1[illegible]:05
                                                                 $(2)   BLANK$COMMON

SYS$*RLIB$. LEVEL [illegible]
END MAP. [illegible]
@XQT
                4.4[illegible]   4.[illegible]   5.[illegible]   [illegible]   [illegible]   7.000000   7.500000   8.000000
  [illegible]   [illegible]   [illegible]   [illegible]   [illegible]   10.400000   10.500000   10.600000
 [illegible]   [illegible]   [illegible]   [illegible]   [illegible]   11.200000   11.300000   11.400000
```

```
 11.500000   11.600000   11.700000   11.800000   11.900000   12.000000   12.100000   12.200000
 12.300000   12.400000   12.500000   12.600000   12.700000   12.800000   12.900000   13.000000
 13.400000   13.700000   14.000000   15.000000   16.000000   17.000000   17.100000     .000170
   .000170     .000750     .000730     .001020     .001550     .002260     .003370     .005150
   .008740     .014390     .034850     .173190     .579070     .902150    1.142100    1.359270
  1.565970    1.753000    1.972070    2.173970    2.395520    2.622470    2.854670    3.126840
  3.414370    3.737010    4.104010    4.572040    5.045930    5.688040    6.525740    7.717420
  9.012470   13.412740   15.494950    2.422700     .972270     .511540     .372470     .116370
   .072790     .050370     .021790     .013790     .010050     .009500
                   Y(T)=  4.000000             ZN(T)=  2.5440279             ZK(T)=   .0001700
                   Y(T)=  5.000000             ZN(T)=  2.1012717             ZK(T)=   .0007500
                   Y(T)=  5.500000             ZN(T)=  2.4414019             ZK(T)=   .0007300
                   Y(T)=  6.000000             ZN(T)=  2.7902715             ZK(T)=   .0010200
                   Y(T)=  7.000000             ZN(T)=  2.3310465             ZK(T)=   .0015500
                   Y(T)=  8.000000             ZN(T)=  2.2544737             ZK(T)=   .0022600
                   Y(T)=  9.000000             ZN(T)=  2.1552075             ZK(T)=   .0033700
                   Y(T)=  9.300000             ZN(T)=  2.0260172             ZK(T)=   .0051500
                   Y(T)=  9.600000             ZN(T)=  1.3410071             ZK(T)=   .0087400
                   Y(T)=  9.800000             ZN(T)=  1.5670000             ZK(T)=   .0143900
                   Y(T)= 10.000000             ZN(T)=  1.0453014             ZK(T)=   .0348500
                   Y(T)= 10.300000             ZN(T)=   .3720000             ZK(T)=   .1731900
                   Y(T)= 10.500000             ZN(T)=   .1770275             ZK(T)=   .5790700
                   Y(T)= 10.600000             ZN(T)=   .1300000             ZK(T)=   .9021500
                   Y(T)= 10.700000             ZN(T)=   .0970507             ZK(T)=  1.1421000
                   Y(T)= 10.750000             ZN(T)=   .0201279             ZK(T)=  1.3592900
                   Y(T)= 10.800000             ZN(T)=   .0371170             ZK(T)=  1.5659700
                   Y(T)= 10.900000             ZN(T)=   .0167075             ZK(T)=  1.7530000
                   Y(T)= 11.000000             ZN(T)=   .0257054             ZK(T)=  1.9720700
                   Y(T)= 11.100000             ZN(T)=   .0350070             ZK(T)=  2.1739700
                   Y(T)= 11.200000             ZN(T)=   .0475070             ZK(T)=  2.3955200
                   Y(T)= 11.300000             ZN(T)=   .0700109             ZK(T)=  2.6224700
                   Y(T)= 11.400000             ZN(T)=   .2777371             ZK(T)=  2.8546700
                   Y(T)= 11.500000             ZN(T)=   .3704143             ZK(T)=  3.1268400
                   Y(T)= 11.600000             ZN(T)=   .1074400             ZK(T)=  3.4143700
                   Y(T)= 11.700000             ZN(T)=   .1247009             ZK(T)=  3.7370100
                   Y(T)= 11.800000             ZN(T)=   .1001210             ZK(T)=  4.1040100
                   Y(T)= 11.900000             ZN(T)=   .1470379             ZK(T)=  4.5720400
                   Y(T)= 12.000000             ZN(T)=   .1707779             ZK(T)=  5.0459300
                   Y(T)= 12.100000             ZN(T)=   .2215040             ZK(T)=  5.6880400
                   Y(T)= 12.200000             ZN(T)=   .4010045             ZK(T)=  6.5257400
                   Y(T)= 12.300000             ZN(T)=   .4607777             ZK(T)=  7.7174200
                   Y(T)= 12.400000             ZN(T)=   .7751130             ZK(T)=  9.0124700
                   Y(T)= 12.500000             ZN(T)=  2.4200000             ZK(T)= 13.4127400
                   Y(T)= 12.600000             ZN(T)=  7.7774777             ZK(T)= 15.4949501
                   Y(T)= 12.700000             ZN(T)= 15.0074145             ZK(T)=  2.4227000
                   Y(T)= 12.800000             ZN(T)= 11.0000000             ZK(T)=   .9722700
                   Y(T)= 12.900000             ZN(T)=  7.0400011             ZK(T)=   .5115400
                   Y(T)= 13.000000             ZN(T)=  7.0700000             ZK(T)=   .3724700
                   Y(T)= 13.400000             ZN(T)=  5.0570040             ZK(T)=   .1163700
                   Y(T)= 13.700000             ZN(T)=  5.4107004             ZK(T)=   .0727900
                   Y(T)= 14.000000             ZN(T)=  4.0000001             ZK(T)=   .0503700
                   Y(T)= 15.000000             ZN(T)=  4.0010000             ZK(T)=   .0217900
                   Y(T)= 16.000000             ZN(T)  7.1000010              ZK(T)=   .0137900
                   Y(T)= 17.000000             ZN(T)  7.1000075              ZK(T)=   .0097500
```

```
@MFOR,LIB.MFOR,IS MAIN
FORTRAN-MACC 1.14S-05/22/79-13:41:10 (,0)        MAIN
00101       1.            DIMENSION R(20),W(20)
00102       2.            EXTERNAL F
00103       3.            COMMON Y1,Z1,Y2,Z2
00104       4.          3 READ(5,7,END=100)WA
00107       5.          7 FORMAT(F5.2)
00110       6.            READ(5,9,END=100)Y2,Z2,Y1,Z1
00116       7.          9 FORMAT(4F10.7)
00117       8.            L=0
00120       9.            CALL NTQUAD(0.0,1.570796,F,20,R,W,L,V,DUM)
00121      10.            VALUE=1.-V
00122      11.            PRINT 200,WA,V,VALUE
00123      12.        200 FORMAT(5X,'WA=',F5.2,24H    SPECTRAL HEMI. EMIT=,E17.7,24H    SPEC
00127      13.           $TRAL HEMI. REF.=,E17.7)
00130      14.            GO TO 3
00131      15.        100 STOP
00132      16.            END

       END OF COMPILATION:        NO  DIAGNOSTICS.
```

```
@MFOR,LIB.MFOR,IS F
FORTRAN-MACC 1.14S-05/22/79-13:41:13 (,0)        F
00101          FUNCTION F(X)
00102          COMMON Y1,Z1,Y2,Z2
00103          C=((Y1*Y2+Z1*Z2)/(Y2**2+Z2**2))*SIN(X)
00104          H=((Y1*Z2-Y2*Z1)/(Y2**2+Z2**2))*SIN(X)
00105          SS=1.-C**2+H**2
00106          TT=2.*C*H
00107          R=(SS**2+TT**2)**0.5
00110          Y=ATAN(-TT/SS)
00111          C=Y1*COS(X)
00112          D=(Y2*COS(Y/2.)+Z2*SIN(Y/2.))*R**0.5
00113          P=Z1*COS(X)
00114          Q=(Z2*COS(Y/2.)-Y2*SIN(Y/2.))*R**.5
00115          S=(C+D)**2+(P+Q)**2
00116          T=C**2-D**2+P**2-Q**2
00117          U=2.*P*D-2.*C*Q
00120          RO1=(T/S)**2+(U/S)**2
00121          C1=Y2*COS(X)
00122          D1=(Y1*COS(Y/2.)+Z1*SIN(Y/2.))*R**0.5
00123          P1=Z2*COS(X)
00124          Q1=(Z1*COS(Y/2.)-Y1*SIN(Y/2.))*R**0.5
00125          S1=(D1+C1)**2+(P1+Q1)**2
00126          T1=D1**2-C1**2+Q1**2-P1**2
00127          U1=2.*Q1*C1-2.*P1*D1
00130          RO2=(T1/S1)**2+(U1/S1)**2
00131          RO=0.5*(RO2+RO1)
00132          E=1.-RO
00133           F=2.*E*SIN(X)*COS(X)
00134          RETURN
00135          END

      END OF COMPILATION:        NO  DIAGNOSTICS.
```

```
@MFOR*LIB.MFOR,IS MAIN
FORTRAN-MACC 1.14S-09/14/79-15:34:44 (,0)        MAIN
00101               DIMENSION EO(44),Y1(44),EB(44),TE(49),FB(44),R(20),W(20),PLAND(44)
00102               EXTERNAL F,FF
00103               COMMON YY,YZ,TT
00104               READ(5,10)(EO(I),I=1,44),(Y1(J),J=1,44)
00116            10 FORMAT()
00117               DO 5 I=1,49
00122               TE(I)=1200.+100.*FLOAT(I-1)
00123               TT=TE(I)
00124               V1=0.
00125               PLAN=0.
00126               DO 2 J=1,27
00131               H=(1.5-0.2)/26.
00132               Y=0.2+H*FLOAT(J-1)
00133               C1=(6.625E-19)*(3.E14)**2
00134               C2=(6.625E-19)*(3.E14)/(1.38E-8)
00135               C3=C2/(Y1(J)*Y*TT)
00136               IF(C3.GT. 85.0)GO TO 2
00140               EX= EXP(C3)-1.
00141               EA=2.*3.141592*C1/(Y1(J)**2*Y**5*EX)
00142               PLAND(J)=EA
00143               PLAN=PLAN+PLAND(J)
00144               EB(J)=EA
00145               V1=V1+H*EO(J)*EB(J)
00146             2 CONTINUE
00150               PLAN=H*(PLAN-0.5*PLAND(1)-0.5*PLAND(27))
00151               V1=V1-0.5*H*(EO(1)*EB(1)+EO(27)*EB(27))
00152               V2=0.
00153               PLA=0.
00154               DO 3 J=27,44
00157               G=(10.-1.5)/17.
00160               X=1.5+G*FLOAT(J-27)
00161               D1=(6.625E-19)*(3.E14)**2
00162               D2=(6.625E-19)*(3.E14)/(1.38E-8)
00163               D3=D2/(Y1(J)*X*TT)
00164               IF(D3.GT. 85.0)GO TO 3
00165               FX= EXP(D3)-1.
00167               FA=2.*3.141592*D1/(Y1(J)**2*X**5*FX)
00170               PLAND(J)=FA
00171               PLA=PLA+PLAND(J)
00172               FB(J)=FA
00173               V2=V2+G*EO(J)*FB(J)
00174             3 CONTINUE
00175               PLA=G*(PLA-0.5*PLAND(27)-0.5*PLAND(44))
00177               PLAN=PLAN+PLA
00200               V2=V2-0.5*G*(EO(27)*FB(27)+EO(44)*FB(44))
00201               YY=Y1(1)
00202               YZ=Y1(44)
00203               L=0
00204               CALL NTGUAD(0.01,0.2,F,20,R,W,L,V,DUM)
00205               V3=EO(1)*V
00206               PLAN=PLAN+V
00207               L=0
00210               CALL NTGUAD(10.,150.,FF,20,R,W,L,V,DUM)
00211               V4=EO(44)*V
00212               PLAN=PLAN+V
```

```
00213      56.             VALUE=(V1+V2+V3+V4)/PLAN
00214      57.             VAL=1.-VALUE
00215      58.             WRITE(6,20)TT,VALUE,VAL
00222      59.          20 FORMAT(5X,'TE= ',F6.1,5X,'TOTAL HEM. EMITTANCE= ',E15.7,5X,
00222      60.            $'TOTAL HEM. REFLECTANCE=',E15.7)
00223      61.             Y1(1)=YY
00224      62.             Y1(44)=YZ
00225      63.           5 CONTINUE
00227      64.             STOP
00230      65.             END

      END OF COMPILATION:        NO  DIAGNOSTICS.
```

```
@MFOR*LIB.MFC2.IS F
FORTRAN-MACC 1.145-09/14/79-15:34:59 (,0)        F
00101       1.              FUNCTION F(X)
00102       2.              COMMON YY,YZ,TT
00103       3.              C1=(6.625E-19)*(3.E14)**2
00104       4.              C2=(6.625E-13)*(3.E14)/(1.38E-6)
00105       5.              IF(X.LT.0.00001)GO TO 6
00107       6.              C3=C2/(YY*X*TT)
00110       7.              IF(C3.GT. 85.0)GO TO 6
00112       8.              GO TO 80
00113       9.           80 IF(C3.LT.1.0E-10)GO TO 6
00115      10.              EX= EXP(C3)-1.
00116      11.              EA=2.*3.141592*C1/(YY**2*X**5*EX)
00117      12.              F=EA
00120      13.              GO TO 7
00121      14.            6 F=0.
00122      15.            7 RETURN
00123      16.              END

      END OF COMPILATION:        NO  DIAGNOSTICS.
```

```
@MFOR*LIB.MFOR.ASIZY FF
FORTRAN-MACC 1.14S-09/14/79-15:35:05 (,0)        FF

   FUNCTION FF          ENTRY POINT 000064

    STORAGE USED:

      0   DATA    000022
      1   CODE    000074

    COMMON BLOCKS:

      2   BLANK$ 000003

    EXTERNAL REFERENCES:

      3   EXP
      4   NERR3$

    STORAGE ASSIGNMENT:

      1   000053 5L           1   000054 7L           1   000023 80L          0 R 000001 C1          0 R 000002 C2
      0 R 000003 C3           0 R 000005 EA           0 R 000004 EX           0 R 000000 FF          0   000015 INJP$
      2 R 000002 TT           2   000000 YY           2 R 000001 YZ


00101      1.             FUNCTION FF(X)
00102      2.             COMMON YY,YZ,TT
00103      3.             C1=(6.625E-19)*(3.E14)**2
00104      4.             C2=(6.625E-19)*(3.E14)/(1.38E-8)
00105      5.             IF(X.LT.0.00001)GO TO 5
00107      6.             C3=C2/(YZ*X*TT)
00110      7.             IF(C3.GT. 85.0)GO TO 5
00112      8.             GO TO 80
00113      9.          80 IF(C3.LT.1.0E-10)GO TO 5
00115     10.             EX= EXP(C3)-1.
00116     11.             EA=2.*3.141592*C1/(YZ**2*X**5*EX)
00117     12.             FF=EA
00120     13.             GO TO 7
00121     14.           5 FF=0.
00122     15.           7 RETURN
00123     16.             END

      END OF COMPILATION:        NO  DIAGNOSTICS.
```

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