Improved Technique for Determining Complex Permittivity with the Transmission/Reflection Method

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Abstract — The transmission/reflection method for complex permittivity and permeability determination is studied. The special case of permittivity measurement is examined in detail. New robust algorithms for permittivity determination that eliminate the ill-behaved nature of the commonly used procedures at frequencies corresponding to integer multiples of one-half wavelength in the sample are presented. An error analysis is presented which yields estimates of the errors incurred due to the uncertainty in scattering parameters, length measurement, and reference plane position. In addition, new equations are derived for determining complex permittivity independently of reference plane position and sample length.

I. INTRODUCTION

Broad-band measurements of complex permittivity and permeability are required for a multitude of applications. Due to its relative simplicity, the transmission/reflection (TR) method is presently a widely used broad-band measurement technique. The relevant literature in this area is copious and no attempt is made in this paper to review it exhaustively. A measurement using the TR method proceeds by placing a sample in a section of waveguide or coaxial line and measuring the two-port complex scattering parameters, preferably by an automatic network analyzer (ANA). The scattering equations then relate the measured scattering parameters to the permittivity and permeability of the material. The system of equations contains as unknowns the complex permittivity and permeability, the calibration reference plane positions, and, in some applications, the sample length. This system of equations is generally overdetermined and therefore can be solved in various ways. From a pragmatic viewpoint, what is needed are equations that are stable over the frequency range of interest and equations that do not depend on the position of the calibration reference plane.

With the development of modern network analyzer systems there is generally no paucity of data; thus correct and efficient numerical algorithms for the reduction of the scattering data are of paramount importance. To accommodate modern network analyzer acquisition systems, Nicolson and Ross [1] and Weir [2] introduced procedures for obtaining broad-band measurements in both time and frequency domains. In the Nicolson–Ross procedure, the equations for the scattering parameters are combined in such a fashion as to allow the system of equations to decouple, yielding an explicit equation for the permittivity and permeability as a function of the scattering parameters. This solution has formed the basis of the commonly utilized technique for obtaining permittivity and permeability from scattering measurements [3]–[5]. The compact form of these equations, while elegant, is not well behaved for low-loss materials at frequencies corresponding to integer multiples of one-half wavelength in the sample. At these frequencies the solution for low-loss materials is divergent. Many researchers have bypassed this problem by using samples which are less than one-half wavelength long at the highest measurement frequency. However, this approach, as shown later in the paper, severely limits the viability of the TR method since short samples increase measurement uncertainty.

Stuchly and Matuszewski [6] presented a slightly different derivation from that of Nicolson and Ross and obtained two explicit equations for the permittivity. They showed that one of these equations was ambiguous; the other equation was similar to the Nicolson–Ross equation which is unstable for low-loss materials at multiples of one-half integer wavelengths. Ligthardt [7], in a detailed analysis, presented a method for shorted line measurements where the scattering equations for the permittivity were solved over a calculated uncertainty region and the results were then averaged. The equations used by Ligthardt are useful for high-loss materials, but for low-loss materials they suffer the same pathologies as the Nicolson–Ross equations at multiples of one-half wavelength. It can be shown that the Nicolson–Ross–Weir solution for combined permeability and permittivity for low-loss materials is inherently divergent at integer multiples of one-half wavelength. In this paper we present a procedure for obtaining complex permittivity from the scattering equations which is stable over the frequency spectrum. This procedure minimizes the instability of the Nicolson–Ross–Weir equations by...
setting $\mu_R = 1$. This new procedure allows measurements to be taken on samples of arbitrary length.

Another problem encountered in practice is the transformation of $S$-parameter measurements from the calibration reference planes to the ends of the sample. This transformation requires knowledge of the position of the sample in the sample holder; however this information may be limited in many applications. The port extension feature of network analyzers is of some help in determining reference plane position, but does not completely solve the problem. Equations that are independent of reference plane positions are desirable. Also, equations that are independent of sample length are useful for high-temperature applications. In the past, other authors addressed the problem of either reference plane invariance or sample length invariance, for example Altschuler [8], Harris [9], and Scott [10], but no one, to our knowledge, has addressed the problem of combined reference plane and sample length invariance.

The goal of this paper is threefold: first, to examine the scattering equations in detail and to present an improved method for solving the transmission line equations in an iterative fashion with application to permittivity measurements; second, to derive scattering equations that are simultaneously invariant to the position of the reference planes and sample length; and, third, to present an uncertainty analysis for this new procedure.

II. THEORY

In the TR measurement technique, a sample is inserted into either a waveguide or a coaxial line and the sample is subjected to an incident electromagnetic field (see Fig. 1). The scattering equations are found from an analysis of the electric field at the sample interfaces. If we assume electric fields $E_1$, $E_{11}$, and $E_{111}$ (with a time dependence of $\exp(j\omega t)$) in the regions I, II, and III, we can write the spatial distribution of the electric field where the incident electric field is 1:

where

$$\gamma = j \sqrt{\frac{\omega^2 \mu_R \varepsilon_R}{\varepsilon_0 c^2}} \left( \frac{2\pi}{\lambda_c} \right)^2$$

$$\gamma_0 = j \sqrt{\frac{\omega}{c_{lab}}} \left( \frac{2\pi}{\lambda_c} \right)^2$$

$$\varepsilon = [\varepsilon_R - j\mu_R] \varepsilon_0 = \varepsilon_R \varepsilon_0$$

$$\mu = [\mu_R - j\mu_R] \mu_0 = \mu_R \mu_0.$$  

Here, $j = \sqrt{-1}$, $c_{vac}$ and $c_{lab}$ are the speed of light in vacuum and in air respectively, $\omega$ is the angular frequency, $\lambda_c$ is the cutoff wavelength, $\varepsilon_0$ and $\mu_0$ are the permittivity and permeability of vacuum, $\varepsilon_R$ and $\mu_R$ are the complex permittivity and permeability relative to a vacuum, and $\gamma_0$ and $\gamma$ are the propagation constants in air and the material respectively. The constants $C_i$ are determined from the boundary conditions. The boundary condition on the electric field is the continuity of the tangential component at the interfaces. The boundary condition on the magnetic field requires the assumption that no surface currents are generated. If this condition holds, then the tangential component of the magnetic field is continuous across the interface. The tangential component of the magnetic field can be calculated from Maxwell’s equations.

For a two-port device the expressions for the measured scattering parameters are obtained by solving (1)-(3) subject to the boundary conditions. Since the $S$ matrix is symmetric, $S_{11} = S_{22}$. The explicit expressions are given by

$$S_{11} = R_1 \left[ \frac{\Gamma(1 - z^2)}{1 - \Gamma^2 z^2} \right]$$

$$S_{22} = R_2 \left[ \frac{\Gamma(1 - z^2)}{1 - \Gamma^2 z^2} \right]$$

$$S_{21} = R_1 R_2 \left[ \frac{z(1 - \Gamma^2 z^2)}{1 - \Gamma^2 z^2} \right]$$

where

$$R_1 = \exp(-\gamma_0 L_1)$$

$$R_2 = \exp(-\gamma_0 L_2)$$

and for coaxial line ($\omega_c \rightarrow 0$) the reflection coefficient

$$\Gamma = \frac{\gamma_0 - \mu}{\gamma_0 + \mu}.$$  

where $L_1$ and $L_2$ are the distances from the calibration reference planes to the sample ends, and $R_1$ and $R_2$ are the reference plane transformation expressions. Of course, (8)-(10) are not new and are derived in detail elsewhere [1], [11]. We define a reflection coefficient by

$$R_1 = \exp(-\gamma_0 L_1)$$

$$R_2 = \exp(-\gamma_0 L_2)$$

$$\Gamma = \frac{\gamma_0 - \mu}{\gamma_0 + \mu}.$$  

and for coaxial line ($\omega_c \rightarrow 0$) the reflection coefficient
reduces to

\[ \Gamma = \frac{c_{\text{vac}}}{c_{\text{lab}}} \sqrt{\frac{\mu R}{\varepsilon R}} - 1 \]

and

\[ \Gamma = \frac{c_{\text{vac}}}{c_{\text{lab}}} \sqrt{\frac{\mu R}{\varepsilon R}} + 1 \]

We also have an expression for \( z \), the transmission coefficient:

\[ z = \exp(-\gamma L) \]

where \( L \) is the sample length. We assume that we know the total length of the sample holder: \( L_{\text{tot}} = L + L_1 + L_2 \). Additionally, \( S_{21} \) for the empty sample holder is

\[ S_{21}^0 = R_1 R_2 \exp(-\gamma_0 L). \]

For nonmagnetic materials, (8), (9), and (10) contain \( \varepsilon R \), \( \mu R \), \( L \), and the reference plane transformations \( R_1 \) and \( R_2 \) as unknown quantities. Since the equations for \( S_{12} \) and \( S_{21} \) are equivalent for isotropic materials, we have four complex equations, (8), (9), (10), and (16), plus the equation for the length of the air line or equivalently, nine real equations for the five unknowns. Additionally, in many applications we know the sample length. For magnetic materials we have seven unknowns. Thus, the system of equations is overdetermined and it is possible to solve the equations in various combinations. As an example, if \( 1/\varepsilon R \) is known accurately, then \( L_1 \) and \( L_2 \) can be eliminated from the equations to obtain equations that are reference-plane invariant. There exists a whole family of reference-plane independent equations and only the most useful are given below as examples:

\[ |S_{21}| = \frac{z(1 - \Gamma^2)}{1 - z^2 \Gamma^2} \]

\[ |S_{11}| = \frac{\Gamma(1 - z^2)}{1 - z^2 \Gamma^2} \]

\[ \frac{S_{11}S_{22}}{S_{12}S_{21}} = \left( \frac{1 - \varepsilon R^2}{4 \mu R^2} \right)^2 \sinh^2 \gamma L \]

\[ \frac{S_{21}}{S_{21}^0} = \exp(\gamma_0 L) \frac{z[1 - \Gamma^2]}{1 - z^2 \Gamma^2} \]

\[ S_{21}S_{12} - S_{11}S_{22} = \exp \left[ (-2\gamma_0)(L_{\text{air}} - L) \right] \frac{z^2 - \Gamma^2}{1 - z^2 \Gamma^2}. \]

Here the vertical bar denotes the magnitude of the complex expression. Equation (19) is valid only for coaxial line. Equation (21) is the determinant of the scattering matrix; the determinant is well known as a quantity invariant to rotations.

Nicolson and Ross [1] and also Weir [2] combined the equations for \( S_{11} \) and \( S_{21} \), (8) and (10), and discovered an explicit formula for the permittivity and permeability. The solution of these equations, however, is not totally straightforward in that an ambiguity in phase must be resolved at each frequency by matching calculated and measured group delay. Also, this procedure does not work well at frequencies where the sample length is a multiple of one-half wavelength in the material. Typical results calculated from the Nicolson–Ross–Weir [1, 2] equations are displayed in Fig. 2 as the solid line. At frequencies corresponding to integer multiples of one-half wavelength in low-loss materials the scattering parameter \( |S_{11}| \) gets very small. The equations are algebraically unstable as \( |S_{11}| \to 0 \); also for small \( |S_{11}| \), the ANA phase uncertainty is large. Since the solution is proportional to \( \frac{1}{\varepsilon_R} \) we see that the phase error dominates the solution at these frequencies. To bypass this problem, many researchers resort to using short samples. However, use of short samples lowers the measurement sensitivity. In fact, as will be shown in Section III, to minimize the uncertainty in low-loss materials a relatively long sample is preferred.

Iterative solution of various combinations of (17)–(21) produces a solution that is stable over the measurement spectrum. Sample length and air line length can be treated as an unknown in the system of equations by solving combinations of (17)–(21). The solution of these equations is then independent of reference plane position, air line length, and sample length. For example, (20) and (21) constitute four real equations that are independent of reference plane; they can be solved as a system with both the sample length and the air line length treated as unknown quantities.

Another interesting result can be obtained if we assume that \( \varepsilon_R \) and the measured value of an \( S \) parameter are known at a single angular frequency, \( \omega_0 \). In this case we can solve either (11) or (12) for the reference positions and then substitute this length into (8)–(10) to obtain relations for the reference plane positions at other fre-
Equations for Numerical Permittivity Determination

There are various ways of solving the scattering equations depending on the information available to the experimenter. For cases where the sample length and reference plane positions are known to high accuracy, we have found that taking various linear combinations of the scattering equations and solving the equations in an iterative fashion yields a very stable solution on samples of arbitrary length. A useful combination is

\[ R_1(\omega_i) R_2(\omega_i) = [S_{21}(\omega_i)]^{(1+\beta)/2} \left[ \frac{1 - z^2 \Gamma^2}{1 - (1 - z^2) \Gamma^2} \right]^{(1+\beta)/2} \]

Thus, we can determine the reference plane positions in terms of \( \varepsilon^\circ_\text{R}(\omega_4) \) and the measured value of the scattering parameter at \( \omega_4 \). Equations (22) and (23) may be very useful for problems where other methods have produced an accurate measurement of \( \varepsilon^\circ_\text{R} \) at a single frequency.

For cases in which the reference plane positions are uncertain, we find that (21) is robust. When using (21) no reference plane transformation need be performed since it has been eliminated by use of the relation \( L_{\text{ref}} = L_1 + L_2 + L \). Equation (21) works well for both low-loss and high-loss materials. If we solve (21) in tandem with any of (17)–(20), we can treat the measurement as independent of reference plane position and sample length.

For magnetic materials, four independent real equations are required (or two independent complex equations). Since in this case we have seven unknowns and nine equations, it is possible to use various combinations of the basic equations (17)–(21); in this case (20) and (21) are recommended. However, for combined permeability and permittivity these equations may not be stable at multiples of one-half wavelength in the sample. To maintain stability another approach is required and results of research will be reported in the near future.

III. Uncertainty Analysis

The sources of error in TR measurement include

- errors in measuring the magnitude and phase of the scattering parameters,
- gaps between the sample and sample holder and sample holder dimensional variations and errors in gap correction formulas,
- uncertainty in sample length,
- line losses and connector mismatch,
- uncertainty in reference plane positions,
- coupling to higher order modes.

The error arising from gaps around the sample can be corrected for in part by using equations available in the literature [12]–[14]. The formulas given in the literature generally undercorrect for the real part of the permittivity and overcorrect for the imaginary part of the permittivity. We assume in the following analysis that all measurements of permittivity have been corrected for air gaps.
around the sample before the following uncertainty analysis is applied. Errors from precision air line dimensional variations have been studied by Hill [15] and it was shown that these uncertainties are generally much smaller than the systematic uncertainty introduced by the network analyzer. In order to evaluate the uncertainty introduced by the measured scattering parameters, a differential uncertainty analysis is applicable, with the uncertainty due to $S_{11}$ and $S_{21}$ evaluated separately. We assume that the total uncertainty can be written as

$$\frac{\Delta \epsilon_R}{\epsilon_R} = \frac{1}{\epsilon_R} \sqrt{\left( \frac{\partial \epsilon_R^s}{\partial |S_{11}|} \Delta |S_{11}| \right)^2 + \left( \frac{\partial \epsilon_R^s}{\partial \theta} \Delta \theta \right)^2 + \left( \frac{\partial \epsilon_R^s}{\partial L} \Delta L \right)^2}$$

and

$$\frac{\Delta \epsilon_T}{\epsilon_T} = \frac{1}{\epsilon_T} \sqrt{\left( \frac{\partial \epsilon_T^s}{\partial |S_{11}|} \Delta |S_{11}| \right)^2 + \left( \frac{\partial \epsilon_T^s}{\partial \theta} \Delta \theta \right)^2 + \left( \frac{\partial \epsilon_T^s}{\partial L} \Delta L \right)^2}$$

where $\alpha = 11$ or 21, $\Delta \theta$ is the uncertainty in the phase of the scattering parameter, $\Delta |S_{11}|$ is the uncertainty in the magnitude of the scattering parameter, and $\Delta L$ is the uncertainty in the sample length. The calculated, $\Delta \epsilon_R^s$, is a worst case estimate. The uncertainty analysis in this section is for the scattering equations in (8)-(10). The derivatives of (8)-(10) can be explicitly calculated. These are given below, assuming $\mu^s = 1$:

$$\frac{\partial \epsilon_R^s}{\partial |S_{11}|} = \frac{[1 - \Gamma^2 z^2] \exp(j\theta)}{Q} \quad (27)$$

$$\frac{\partial \epsilon_R^s}{\partial \theta} = j |S_{21}| \frac{\partial \epsilon_R^s}{\partial |S_{21}|} \quad (28)$$

\[
\left( \frac{\partial \epsilon_R^s}{\partial L} \right)_{S_{21}} = -C \left[ (1 - \Gamma^2) + 2S_{21} \Gamma^2 z \right] \quad (29)
\]

where

$$Q = 2A \Gamma z [S_{21} z - 1] + B [1 - \Gamma^2] + 2S_{21} \Gamma^2 z \quad (30)$$

$$A = \frac{\omega^2}{2 \gamma_0 \epsilon_{\text{vac}}^2} \left[ \frac{1}{1 + \frac{\gamma}{\gamma_0}} \right] \left[ \frac{1 - \gamma}{1 + \frac{\gamma}{\gamma_0}} \right] \quad (31)$$

$$B = \frac{L \omega^2 z}{2 \epsilon_{\text{vac}}^2 \gamma} \quad (32)$$

$$C = -\gamma z \quad (33)$$

$$\left( \frac{\partial \epsilon_T^s}{\partial |S_{11}|} \right)_{S_{11}} = \frac{[1 - \Gamma^2 z^2] \exp(j\theta)}{P} \quad (34)$$

$$\left( \frac{\partial \epsilon_T^s}{\partial \theta} \right)_{S_{11}} = j |S_{11}| \frac{\partial \epsilon_T^s}{\partial |S_{11}|} \quad (35)$$

\[
\left( \frac{\partial \epsilon_T^s}{\partial L} \right)_{S_{11}} = \frac{2C \Gamma [1 - S_{11} \Gamma]}{P} \quad (36)
\]

where

$$P = A \left[ (1 - z^2) + 2S_{11} z^2 \Gamma \right] + 2B \Gamma z \left[ S_{11} \Gamma - 1 \right]. \quad (37)$$

The measurement bounds for $S$-parameter data are obtained from specifications for a network analyzer. The dominant uncertainty is in the phase of $S_{11}$ as $|S_{11}| \to 0$. The uncertainty in $|S_{21}|$ is relatively constant until $|S_{21}| \leq -40$ dB; it then increases abruptly. In Figs. 4–9 the total uncertainty in $\epsilon_R^s$, $\epsilon_T^s$, calculated from $S_{21}$ and $S_{11}$ is plotted as a function of normalized sample length for coaxial low-loss and high-loss materials at 3 GHz with various values of $\epsilon_R^s$ and the guided wavelength in the

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1. Trade names are included in order to allow the reader to duplicate the $S$-parameter uncertainties. Inclusion does not imply endorsement by the National Institute of Standards and Technology.
Fig. 6. The relative uncertainty in $\varepsilon_f(\omega)$ for $S_{21}$ from (25) as a function of frequency for a high-loss material as a function of normalized length, with $\varepsilon_f = (5.0, 2.0)$ in solid line and $(10.0, 2.0)$ in dashed line. The S-parameter uncertainties are the same as in Fig. 4. (See footnote 1.)

Fig. 7. The relative uncertainty in $\varepsilon_f(\omega)$ for $S_{21}$ from (26) as a function of frequency for a high-loss material as a function of normalized length, for $\varepsilon_f = (5.0, 2.0)$ in solid line and $(10.0, 2.0)$ in dashed line. The S-parameter uncertainties are the same as in Fig. 4. (See footnote 1.)

Fig. 8. The relative uncertainty in $\varepsilon_h(\omega)$ for $S_{11}$ from (25) as a function of frequency for a high-loss material as a function of normalized length with $\varepsilon_f = (5.0, 5.0)$ in solid line and $(10.0, 5.0)$ in dashed line. The S-parameter uncertainties are the same as in Fig. 4. (See footnote 1.)

Fig. 9. The relative uncertainty in $\varepsilon_h(\omega)$ for $S_{11}$ from (26) as a function of frequency for a high-loss material as a function of normalized length with $\varepsilon_f = (5.0, 5.0)$ in solid line and $(10.0, 5.0)$ in dashed line. The S-parameter uncertainties are the same as in Fig. 4. (See footnote 1.)

material given by

$$\lambda_m = \frac{2\pi}{\sqrt{\omega^2 \left( \sqrt{\epsilon_f^2 + \mu_f^2 + \epsilon_f} \right) - \frac{2\pi}{\lambda_c^2}}}. \quad (38)$$

We see that the minimum uncertainty for low-loss materials occurs at multiples of one-half wavelength. The reason for this can be determined from examination of (8) and (10) in the limit where $|S_{11}| \to 0$, $|S_{21}| \to 1$ with $\Gamma \neq 0$. These equations then reduce to

$$z^2 - 1 \to 0. \quad (39)$$

Generally, we see a decrease in uncertainty as a function of increasing sample length. In the case of $S_{21}$ for high loss as shown in Figs. 6 and 7, we see first a general decrease in uncertainty and then an increase in uncertainty. This increase occurs because $\Delta|S_{21}|$ increases when the transmitted signal is less than $-40$ dB from the reference. For the case of high loss, the uncertainty in $S_{11}$ approaches a constant value. This is so because, for high-loss materials where the wavelength is much smaller than the sample length, only weak signals penetrate through the sample and thus the front face reflection dominates the $S_{11}$ parameter. In Figs. 8 and 9 we note a number of peaks. These peaks occur when (37) gets very small. Also, the uncertainties in the $S$ parameters have some frequency dependence, with higher frequencies having larger uncertainties in phase. In Fig. 10 a measurement of heavy metal fluoride glass is presented with uncertainty bounds. Note that the peaks of uncertainty coincide with the peaks in the measurement noise. Also note that the uncertainties are quite conservative. This is
due to the conservative estimate of the manufacturer for the S-parameter uncertainty. When (21) is used for permittivity determination, uncertainties in both $S_{21}$ and $S_{11}$ must be included in (25).

Another important source of error is the uncertainty in the location of the reference planes. Generally, when TR experiments are carried out, the sample is placed flush with the end of the sample holder and hence coincident with a calibration reference plane. This placement procedure leaves room for positioning errors, particularly when the sample is loose. The error introduced by incorrect positioning of the sample can be estimated in terms of the error in the reference plane transformation terms (11) and (12). If we have an uncertainty of $\Delta L_1$ in the sample position, then

$$S_{11} = R_{11} S_{11} e^{i\theta} = |S_{11}| \exp \left[ i \theta - 2 \gamma_0 (L_1 + \Delta L_1) \right]. \tag{40}$$

The error in the measured angle is given by

$$\Delta \theta = 2 \gamma_0 L = 4 \pi \frac{\Delta L}{\lambda_{air}}. \tag{41}$$

Therefore small reference plane positioning errors can, in principle, introduce large uncertainties in the $S_{11}$ phase at high frequencies. One way to minimize this is to use equations that are invariant to reference plane position.

IV. DISCUSSION AND CONCLUSIONS

As we have seen, although the Nicolson–Ross–Weir approach is easy to implement numerically, it fails as a solution technique for broad-band measurement of low-loss samples of arbitrary length. The solution presented in this paper uses a Newton–Raphson iteration procedure on combinations of the scattering parameters. This procedure yields solutions that are stable at integer multiples of one-half wavelength in the sample; at the same time it does not unduly increase the complexity of the numerical solution. For materials where the transmitted signal is more than $-40 \text{dB}$ from the reference signal, it is suggested that $S_{21}$ data by themselves are sufficient to calculate permittivity. For materials of large attenuation, $S_{11}$ by itself will produce optimal results. In general, we have found (21) to be robust for high-loss and low-loss materials. The problem of reference plane position has been addressed, and approaches for the minimization of the error have been presented. Equations that are independent of reference plane position and sample length have been presented. Equations that are independent of plane position should be very useful in elevated temperature applications. Generally, sample length can be measured with great accuracy at laboratory temperature, and for these problems it is preferable to use a measured length. However, in temperature-dependent applications it may be better to use equations independent of both sample length and reference plane position.

An uncertainty procedure has been presented for the solution method expounded in this paper. The uncertainty analysis presented here differs in some respects from what has been presented in the literature previously. This difference is due primarily to the fact that the uncertainties in this paper are derived from $S_{11}$ and $S_{21}$ in isolation. The trend indicates that for low-loss materials the uncertainty decreases as a function of increasing sample length. For high-loss materials the uncertainty in $S_{21}$ decreases until the signal reaches $-40$ to $-50 \text{dB}$, and thereafter the uncertainty increases and thus $\Delta \epsilon^R$ increases.

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REFERENCES


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