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Reconstruction of the Constitutive Parameters for Composite Media Using Kramers - Kronig Analysis

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Abstract

An alternative method of determining of the constitutive dispersion parameters for composite media is discussed. It is assumed, that the constitutive materials of composite media are characterized by the complex dielectric permittivity. Furthermore, we consider the composite media with small inclusions as compared with the wavelength of that range for which the dispersion parameters are determined. We have used the experimental reflectance spectra of the composite media from which the effective complex optical refractive index and effective complex dielectric permittivity were determined.

1. Introduction

Last time considerable attention has been devoted on the inverse problem of determining the constitutive parameters of complex media [1-3]. Sometimes using of general methods for determining the constitutive parameters of such media, e.g. solutions of biological macromolecules in aqueous media, is restricted by strong absorption of water outside the transparent ranges. To overcome this problem an alternative method of Kramers-Kroning analysis of the experimental spectra can be applied [3]. In this work, the effective optical functions $\tilde{n}$ and $\tilde{k}$, were obtained using Kramers-Kroning analysis from the experimental reflectance spectra of the composite medium. The real and imaginary parts of the effective complex dielectric permittivity $\tilde{\varepsilon}$ were calculated using the effective optical functions.

2. Theory

The complex reflection amplitude of a normal incident electromagnetic wave, used in the Kramers-Kronig analysis, is defined as follows [1]

$$\tilde{R}^{1/2} = \frac{(\tilde{n}-1)+i\tilde{k}}{(\tilde{n}+1)+i\tilde{k}} = R^{1/2}e^{i\varphi} \tag{1}$$

were R is the magnitude of the reflectance at the frequency ω. The phase φ is related to the reflectance by the dispersion equation, defined in the Kramers-Kronig analysis as follows

$$\varphi(\omega) = \frac{\omega}{\pi} P\int_0^{\infty} \frac{\ln R(\xi)}{\xi^2-\omega^2} d\xi - \pi \tag{2}$$

were P stands for the Cauchy principal value. The real and imaginary parts of the complex optical refractive index $\tilde{n}$ and $\tilde{k}$ are related to the reflectance amplitude and phase by the relations

$$\tilde{n}=\frac{1-R}{1+R+2R^{1/2}\cos\varphi},\qquad \tilde{k}=\frac{-2R^{1/2}\sin\varphi}{1+R+2R^{1/2}\cos\varphi} \tag{3}$$

Using obtained complex refractive index we can calculate the real and imaginary parts of the effective dielectric permittivity of the composite medium $\tilde{\varepsilon}_1=\tilde{n}^2-\tilde{k}^2, \tilde{\varepsilon}_2=2\tilde{n}\tilde{k}$. Further, using the effective complex permittivity of the composite medium, we can obtain the complex dielectric permittivity of the constituents. For this purpose we can utilize one of the widely used approximations, such as Maxwell-Garnett or Bruggeman formalism

$$\tilde{\varepsilon}_{MG}=\varepsilon_h+3f\varepsilon_h\frac{\varepsilon_i-\varepsilon_h}{(1-f)\varepsilon_i+(2+f)\varepsilon_h},\quad f\frac{\varepsilon_i-\tilde{\varepsilon}_{BG}}{\varepsilon_i+2\tilde{\varepsilon}_{BG}}+(1-f)\frac{\varepsilon_h-\tilde{\varepsilon}_{BG}}{\varepsilon_h+2\tilde{\varepsilon}_{BG}}=0 \tag{4}$$

were ε_i is the dielectric permittivity of the inclusions, ε_h is the dielectric permittivity of the host medium. Using known dielectric parameters of the host and the filling factor for the inclusions, we can reconstruct the dielectric permittivity for the inclusions, or using known dielectric permittivity of the inclusions and host medium we can determine the filling factor of the inclusions.

3. Numerical results

To demonstrate the validity of the above formalism the composite structure was considered in a mixture form of LiF small particles embedded in a KBr host. The optical constants for LiF particles correspond to the classical oscillator theory. The relevant real and imaginary parts of the complex dielectric permittivity have the following form

$$\varepsilon'=n^2-k^2=\varepsilon_\infty+\sum_j\frac{4\pi\rho_j\omega_j^2\left(\omega_j^2-\omega^2\right)}{\left(\omega_j^2-\omega^2\right)^2+\left(\gamma_j\omega_j\right)^2},\quad \varepsilon''=2nk=\sum_j\frac{4\pi\rho_j\omega_j^2\left(\gamma_j\omega_j\right)}{\left(\omega_j^2-\omega^2\right)^2+\left(\gamma_j\omega_j\right)^2} \tag{5}$$

The experimental reflectance spectra, taken from the literature [5], for the composite structure with filling factor $f=0.2$ is shown on Fig.1. The calculated phase using Kramers-Kroning analysis is shown on same Fig.1. The effective optical constants of LiF-KCl composite, calculated using Kramers-Kroning, are shown on Fig.2. The experimental and restored effective complex dielectric permittivity for LiF-KCl composite are shown on Fig.3. Finaly, the restored real and imaginary parts of the complex dielectric permittivity of the inclusions are shown on Fig. 4.

4. Conclusion

The apparent conformity of restored complex effective dielectric permittivity with experimental curves proves the validity of above formalism. This rather simple procedure will be useful for spectroscopic investigation of complex media, e.g. in spectroscopic studying of biological macromolecules immersed in aqueous solutions with known dispersion properties.

References

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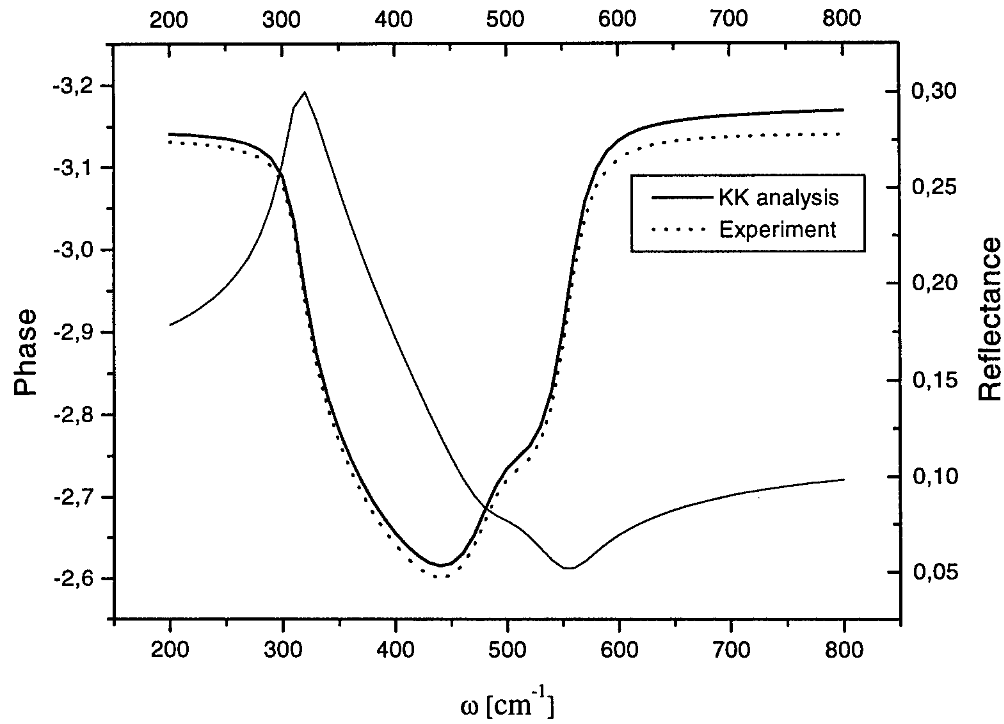

Fig. 1 Reflectance spectra and restored faze of reflected wave for LiF particles embedded in KBr host.

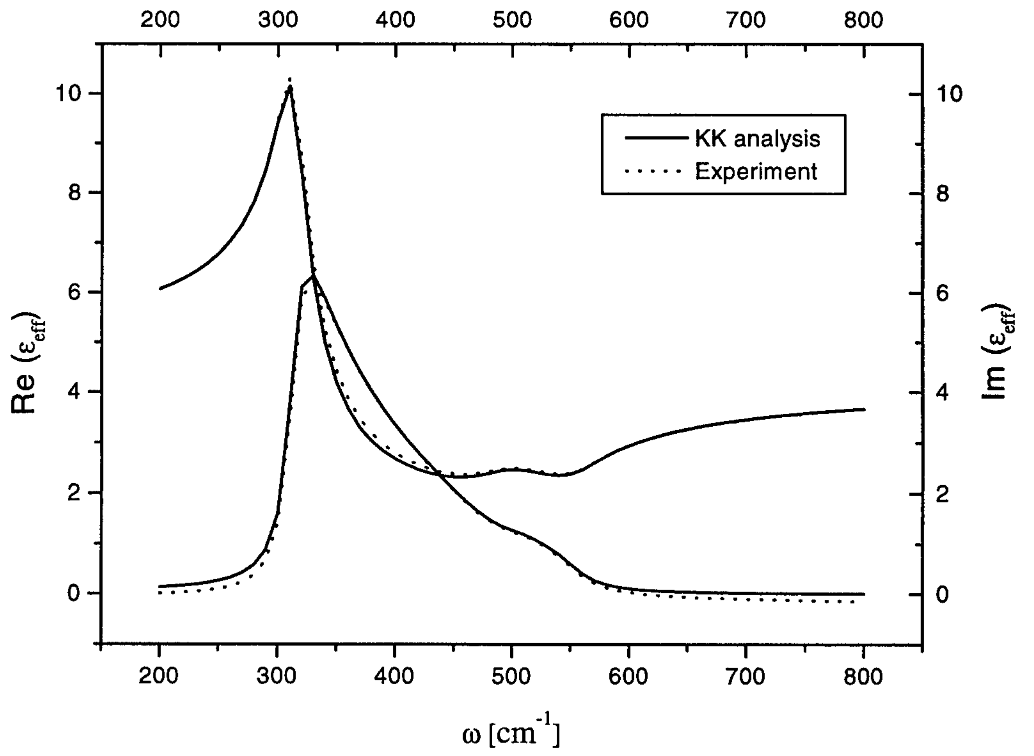

Fig. 2 Restored real and imaginary parts for the effective dielectric permittivity.

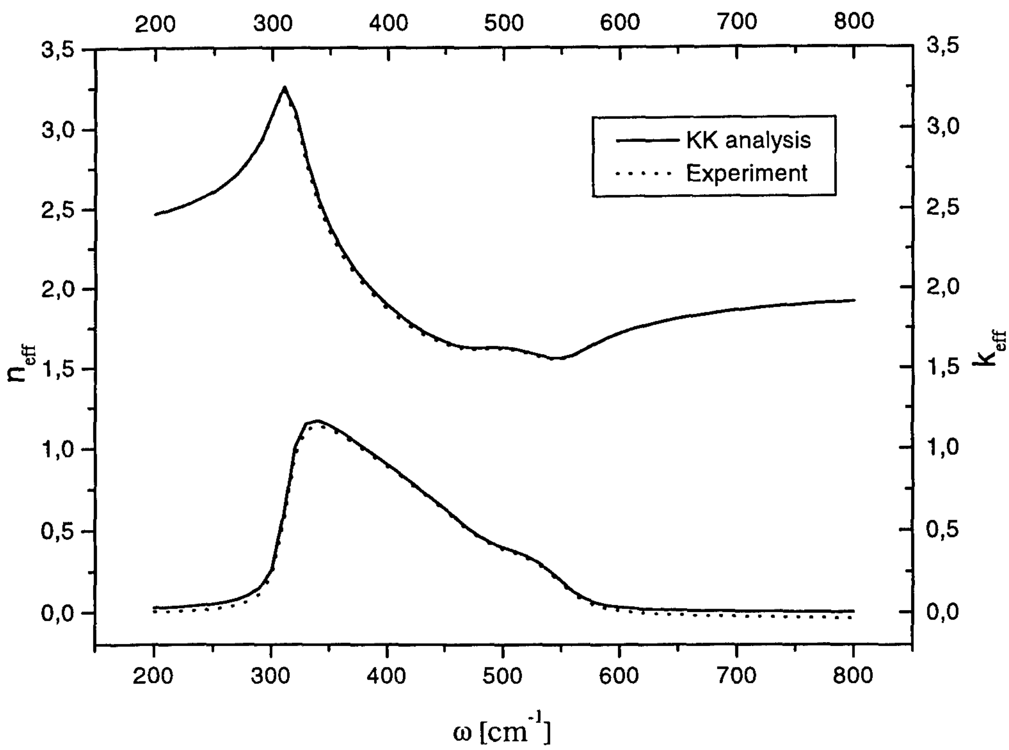

Fig. 3 Restored real and imaginary parts of the complex effective optical functions

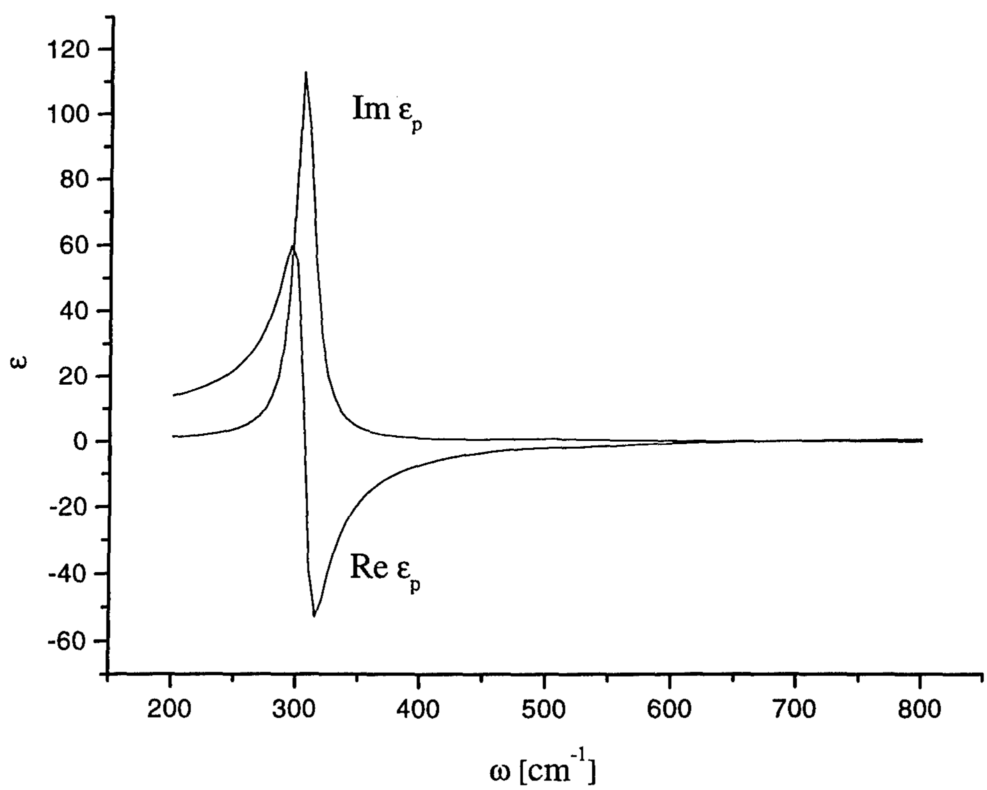

Fig. 4 Restored real and imaginary parts of the dielectric permittivity of the inclusions.