

On the Dielectric Function of Partially Amorphous Olivine Dust

David K. Lynch and S. Mazuk

The Aerospace Corporation, P.O. Box 92957, Los Angeles, CA 90009

Abstract. We present a new technique for computing the optical constants for partially disordered solids based on their crystalline optical constants. The technique assumes that the material is composed of a continuous distribution of oscillators (CDO) and that the degree of atomic disorder can be described by one, or at most two, scalar parameters. We apply the technique to an oft-mentioned solar system material, olivine, and show that its dielectric functions can be predicted for an arbitrary degree of disorder.

1. Introduction

For twenty five years astronomers have puzzled over the smoothness of the 9.7 μm silicate feature that is observed in many cosmic sources. In the laboratory, the features bristle with fine structure that correlates with mineralogical composition and provides a basis for identification. One explanation for the cosmic feature's unstructured spectrum is that the silicates are amorphous (glassy). Spectra of glassy materials show far less spectral structure than the crystalline version and it follows that the optical constants must also be smoother. Yet dielectric functions are seldom measured for amorphous materials and there is no generally available means of computing them theoretically. What is needed, then, is a means of describing an amorphous material's optical properties, primarily in the infrared. The goal of this paper is to analytically simulate the effects of atomic disorder of an arbitrary material.

2. Single and Multiple Oscillators (Lorentz's Classical Model)

In Lorentz's classical model of a damped harmonic oscillator of mass m , spring constant K and damping parameter b , the dielectric function $\epsilon(\omega) = \epsilon' + i \epsilon''$ is given by

$$\epsilon(\omega) = 1 + \omega_p^2 / (\omega_o^2 - \omega^2 - i \gamma_o \omega) \quad (1)$$

where ω_o is the resonant frequency $(K/m)^{1/2}$, γ_o is the damping constant b/m , and ω_p is the plasma frequency Ne^2/m (Bohren and Huffman 1983). N is number of atoms per unit volume and e is the electric charge. For a homogeneous mixture of M different oscillators, the dielectric function is a linear superposition of the individual dielectric functions

$$\epsilon = \overline{\epsilon_0} + \sum_j^M (\omega_p^2)_j / (\omega_j^2 - \omega^2 - i \gamma_j \omega) \quad (2)$$

where $\overline{\epsilon_0}$ is the mean static dielectric constant.

3. Continuous Distribution of Oscillators (CDO) Approximation

We shall make the assumption that a continuous distribution of oscillators (CDO) is equivalent to a homogeneous mixture of oscillators (Equation 2) and that the summation in Equation 2 can be replaced by an integral.

$$\hat{\epsilon}(\omega) = \overline{\epsilon_0} + \iint F(\omega_0 - \omega_0', \gamma_0 - \gamma_0') (\omega_p^2) / (\omega_0'^2 - \omega^2 - i \gamma_0 \omega) d\omega_0' d\gamma_0' \quad (3)$$

where $\hat{\epsilon}(\omega)$ is the dielectric function of the partially crystalline material whose crystalline dielectric function is represented by $\epsilon(\omega)$ or equation 1. $F(\omega, \gamma)$ is the number distribution of oscillators. (In the virtually identical quantum mechanical version of the dielectric function, F includes the oscillator strength.) Equation (3) is a generalization of equation (2) and therefore satisfies the Kramers-Kronig relation. The simplest case of a glassy version of an otherwise crystalline material is one in which the distribution of resonance frequencies is symmetric about the original resonant frequency ω_0 . The function form of equation (3) is equivalent to a filter $F(\omega, \gamma)$ that is convoluted with the crystalline dielectric function. If we integrate over frequency space only, then the operator has the form

$$\hat{\epsilon}(\omega) = \overline{\epsilon_0} + \int F(\omega_0 - \omega_0') (\omega_p^2) / (\omega_0'^2 - \omega^2 - i \gamma_0 \omega) d\omega_0' \quad (4)$$

where the filter function $F(\omega)$ can be any suitable function such as a gaussian.

4. Application of CDO to Olivine

Steyer (1974) measured the three components of $\epsilon(\omega)$ corresponding to the principal axes of the orthorhombic olivine crystal. A sample from the same piece of olivine was bombarded with 1.5 MeV neon atoms to produce a "disordered" form of the mineral by Krättschmer and Huffman (1979). Its dielectric function $\hat{\epsilon}(\omega)$ was then measured (Figure 1, vertical lines). Following Equation (4) we filtered Steyer's three dielectric functions using a rectangular Π_Δ filter with a width of 90 cm^{-1} , then averaged them. No vertical scaling or normalization was done nor did we filter in damping (γ) space. The computed dielectric functions $\hat{\epsilon}(\omega)$ are compared to Krättschmer and Huffman's in Figure 1 (dotted lines). We performed trial-and-error tests until our results were close to those of K& H as judged by eye. The agreement between experiment and theory is encouraging, especially in view of the simplicity of the CDO approximation and the fact that only a single free parameter - the filter width Δ - was used in the fit. Based on this demonstration, we believe that CDO constitutes a useful and versatile first approximation of the dielectric function of amorphous materials. The technique is most applicable to strong resonances in the infrared, i.e., where incoming photons excite phonons

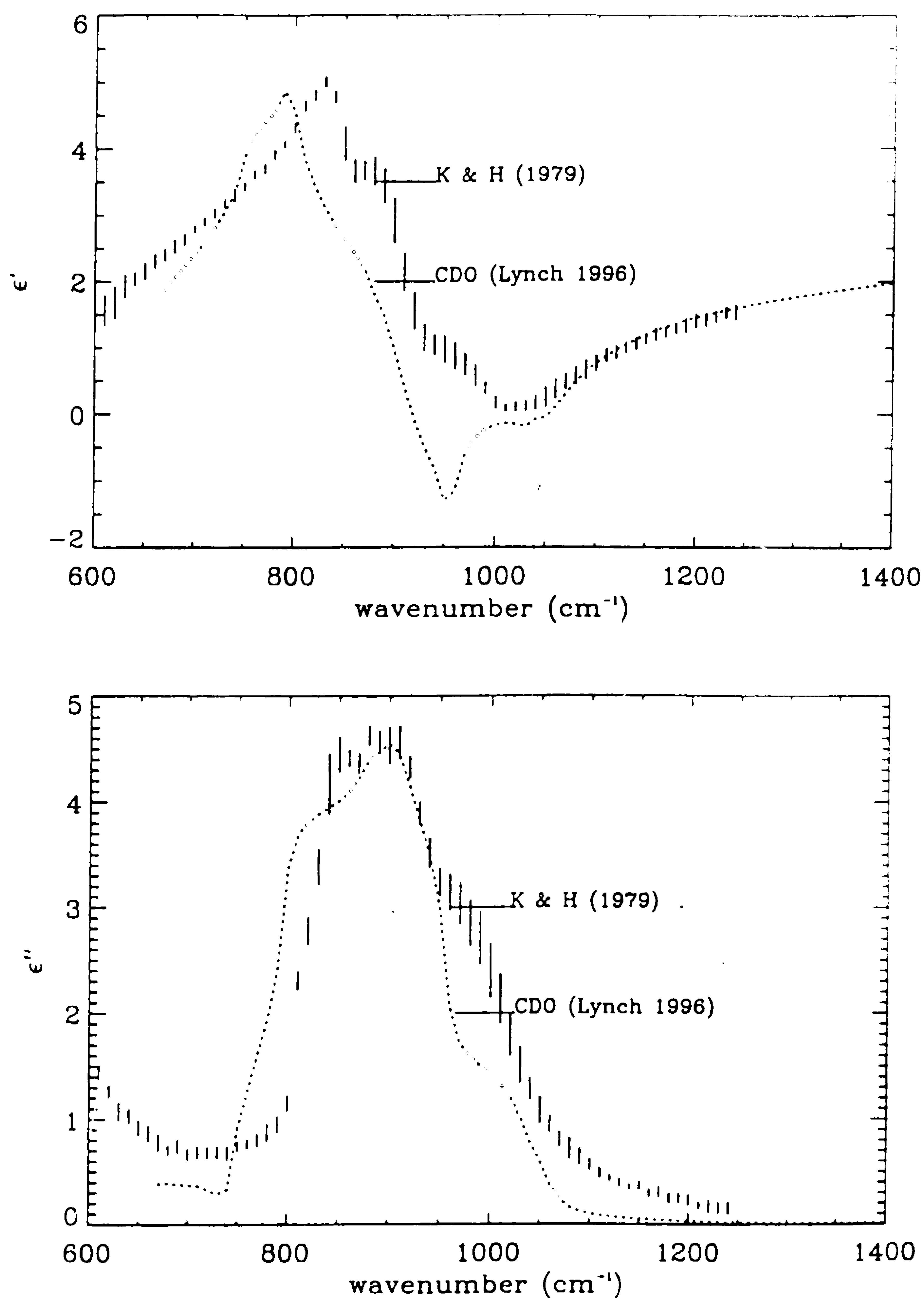


Figure 1. Krätshmer and Huffman's (K&H) measured dielectric function $\hat{\epsilon}(\omega)$ of amorphous olivine (vertical lines), and continuous distribution of oscillators (CDO - Lynch 1996) prediction of the dielectric function based on Steyer's dielectric functions and a Π_{Δ} filter width of 90 cm^{-1} . Upper: real part, Lower: imaginary part.

7. Conclusion

A new technique for approximating the dielectric function of partially crystalline material based on the dielectric function of the crystalline form of the material is presented. This is done by low pass filtering the crystalline dielectric function. The technique is based on a simple extension of the Lorentz theory in the form of a low pass filter. The resulting dielectric functions satisfy the Kramers-Kronig dispersion relations. Comparisons of laboratory and theoretical dielectric functions for olivine show the technique to reproduce measured data with reasonable accuracy.

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References

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