Finding Conductivity and Dielectric Functions by Kramers-Kronig Analysis

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Abstract

In this article we want to review the interesting analysis that should be done on experimental information about normal reflectivity of a material to find its conductivity and dielectric functions. We also will briefly review the experiments apparatus.

INTRODUCTION

We can extract inftyormation about the electronic structure of a solid by studying its conductivity and dielectric functions. Our goal here is to see how we can find these two functions. First, using Maxwell's equations, we will see that it is very natural to construct a complex function, $\epsilon(\omega)$, from these two functions of frequency. They will be proportional to imaginary and real parts of ϵ. Using boundary conditions in Maxwell's theory we can relate this function to $r(\omega)$ the ratio of reflected and initial electric fields which is another complex function of frequency. Reflectivity is the square of the absolute value of $r(\omega)$. It is a real function $R(\omega)$ and is measurable.
So we can measure the modulus of $r(\omega)$. Fortunately, causality is a constraint that gives the inftyormation about phase of $r(\omega)$, if we know its modulus over all frequencies. This is called Kramers Kronig analysis. But we can measure $R(\omega)$ only for a finite interval of frequency, so we have to use models and extrapolations to find R on other parts of the frequency axis. We will briefly mention some of these models.
The only remaining part of the project is to measure $R(\omega)$. It is not a trivial experiment, so we will review some analysis that is involved here as well as the apparatus that is used.

1 - Maxwell's theory relates $R(\omega)$ to $\epsilon(\omega)$

Using Maxwell's equationswe find that the electric field satisfies :
$\nabla^2 E = \frac{\epsilon\mu}{c^2}\frac{\partial^2}{\partial t^2}E + \frac{4\pi\sigma\mu}{c^2}\frac{\partial}{\partial t}E$ [1]
Assuming space time dependence of the form :
$E = E_0 exp(\frac{-k\omega}{c}e_3.r) expi(\frac{n\omega}{c}e_3.r - \omega t)$ [2]
We will find that $(n + ik)^2 = \mu(\epsilon_1 + i\epsilon_2)$ [3]
in which
$\epsilon_1 = \epsilon$ [4]
$\epsilon_2 = \frac{4\pi\sigma]}{\omega}$ [5]

So having ϵ and σ, we can find n and k .
The reflection coefficient in terms of these parameters is
$R = |r|^2$ [6]

$r = \frac{E_r}{E_i} = \frac{1-ik-n}{1+ik+n} = \rho e^{i\theta}$ [7]

All parameters in these formulas are functions of frequency.

2-Causality and Kramers-Kronig relations

$r(\omega)$ has neither zero nor pole in the upper half of the complex plane. (r=0 means n=1 and k=0, which are characteristics of vacum. Being analytic is a consequence of causality.)

So $ln(r) = ln(\rho) + i\theta$ is analytic in the upper half of the complex plane . As a result

$\theta(\omega_0) = \frac{2\omega}{\pi}\int_0^\infty \frac{Ln(\frac{\rho(\omega)}{\rho(\omega_0)})}{\omega_0^2-\omega^2}d\omega = \frac{\omega}{\pi}\int_0^\infty \frac{Ln(\frac{R(\omega)}{R(\omega_0)})}{\omega_0^2-\omega^2}d\omega$ [8]

Using relation [8] we can find $\theta(\omega)$, then using [7] we can find $r(\omega)$, $n(\omega)$, $k(\omega)$, then using [3] we can find $\epsilon_1(\omega)$ and $\epsilon]_2(\omega)$, then using [4] and [5] we can find $\epsilon(\omega)$ and $\sigma(\omega)$.

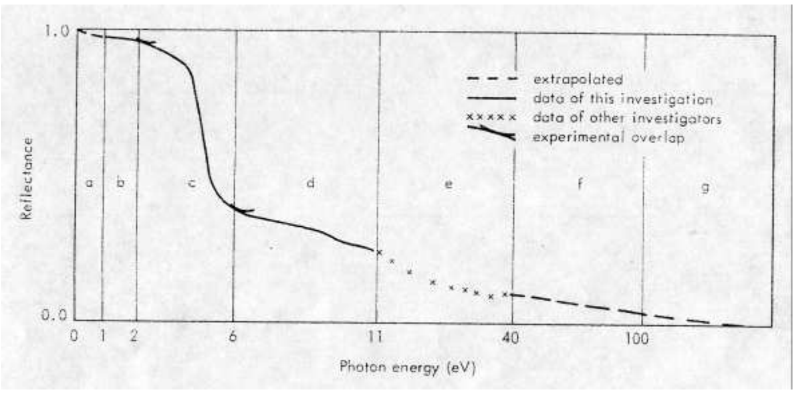

Figure 1: *Idealized composite reflectance curve. Spectral regions: (a) low-energy, linear extrapolation of data from region (b); (b) near-infrared; (c) visible and ultraviolet; (d) vacuum-ultraviolet; (e) data from other investigators; (f) empirical power-law extrapolation; (g) free electron gas asymptotic reflectance extrapolation. [1].*

3- Assumptions about $R(\omega)$.

In order to use relation [8], we need to assume some value for $R(\omega)$ in the region that we cannot measure it. For very high frequencies we will use Lorenz- Drude model's prediction:

$\epsilon = 1 + \frac{a}{-i\Gamma\omega - \omega^2 + \omega_0^2}$[9]
for $\omega \gg \omega_0$ we conclude:

$\epsilon = 1 - \frac{a}{\omega^2}$[10]
Using [10] , [3] with $\mu = 1$, [7] and $\omega \gg \omega_0$, we conclude:

$r = \frac{b}{\omega^2}$ [11]

and using [6] we will have

$R = \frac{c}{\omega^4}$ [12]

Between the very high frequency region and the interval that we measure R, we still assume a power-law dependence on frequency, but with power -s instead of -4:
$R = \frac{d}{\omega^s}$ [13]

s and other free parameters will be chosen to give the best result for the optical constants.

If the sample is a metal we want $R \to 1$ as $\omega \to 0$. If it is not metal, we may extrapolate R linearly to $\omega = 0$.

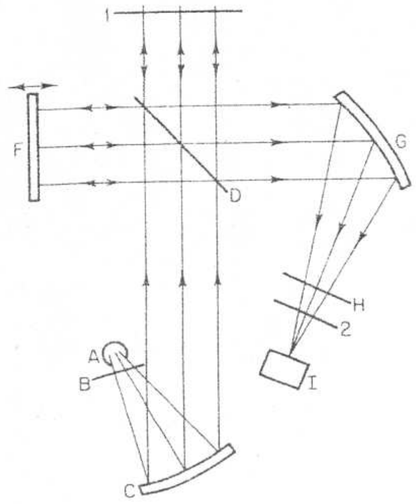

Figure 2: *Basic Michelson Interfereometer. A:Source. B: Chopper. C: Collimator. D: Beamsplitter. E: Fixed mirror. F: Movable mirror. G:Focousing mirror. H: Spectral filters. I: Detector. [2].*

4- The experiment.

To measure the reflectivity of a sample we use Michelson's interferometer. Fig. 2 shows a schematic diagram of Michelson's interferometer."
"The source is black body radiation at about T= 1200 K with a filter that cutts off high frequecies. A chopper modulates the source radiation with a frequency so that we can distinguish the background from useful data by amplifying that frequency. If we put our sample in place of mirror G, we will get the data for oblique incidence.If we are interested in normal incidence reflection, instead of one single mirror G, we will use a set of mirrors to send light perpendicular to our sample. The detector here is a Bolometer.
The direct output of this experiment is the intensity of the reflected light as a function of x, the position of the movable mirror.

$I_0(x) = \int s(\omega)R(\omega)(1 + cos(\frac{2\omega}{c}x))d\omega$ [14]

Here S is the intensity distribution of the source. We find S by replacing the sample with a mirror. In that case:

$I(x) = \int s(\omega)(1 + cos(\frac{2\omega}{c}x))d\omega$ [15]

5- Extracting R from I

If we have I(x) for all values of x, we can Fourier transform it, and find $S(\ omega)R(\omega)$ and

$S(\omega)$.

$R(\omega) = \frac{R(\omega)S(\omega)}{S(\omega)} = \frac{\int I(x)cos(\frac{2\omega}{c}x)dx}{\int I_0(x)cos(\frac{2\omega}{c}x)dx}$ [16]

Of course we cannot integrate x from $-\infty$ to ∞ because we have I(x) only in a finite interval. In order to reduce the effect of finite integration (beside mathematical technics called appodizing) we use a filter to exclude high frequencies from the spectrum of the source. When we have finite integration over x, frequency components other than ω will contribute to ω , so we will exclude them by a filter.

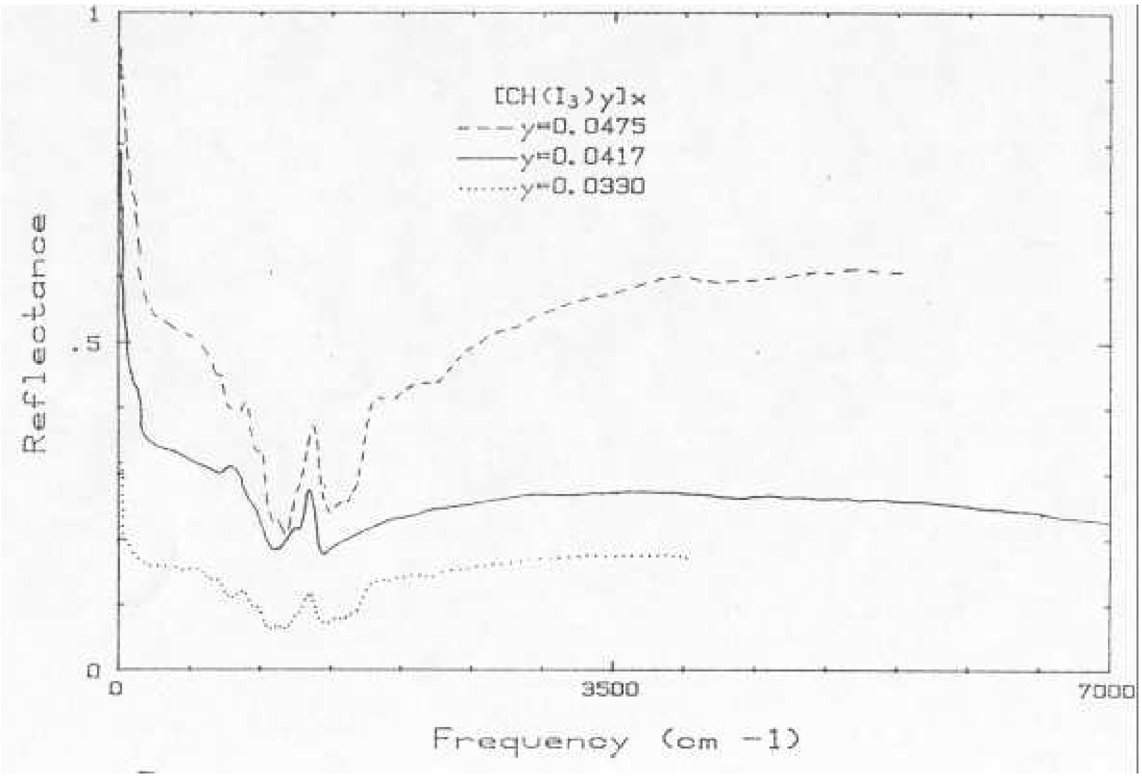

Figure 3: *Reflectance of heavily iodine doped polyacetylene [3].*

6- Concolusion

In this article we investigated one way of measuring optical properties of a solid like ϵ_1 and ϵ_2 The Apparatus of measurement gave us an intensity function I(x).Then by Fourier analysis of I(x), we found $R(\omega)$.Using causality condition we recovered the phase change of reflected light, so we recovered a complex function $r(\omega)$.Boundary conditions in Maxwell's theory relates this $r(\omega)$ to $\epsilon(\omega)$ and by looking at real and imaginary parts of this function we can find dielectric and conductivity functions. Fig.3, 4 and five show a few resuls of this experiment.

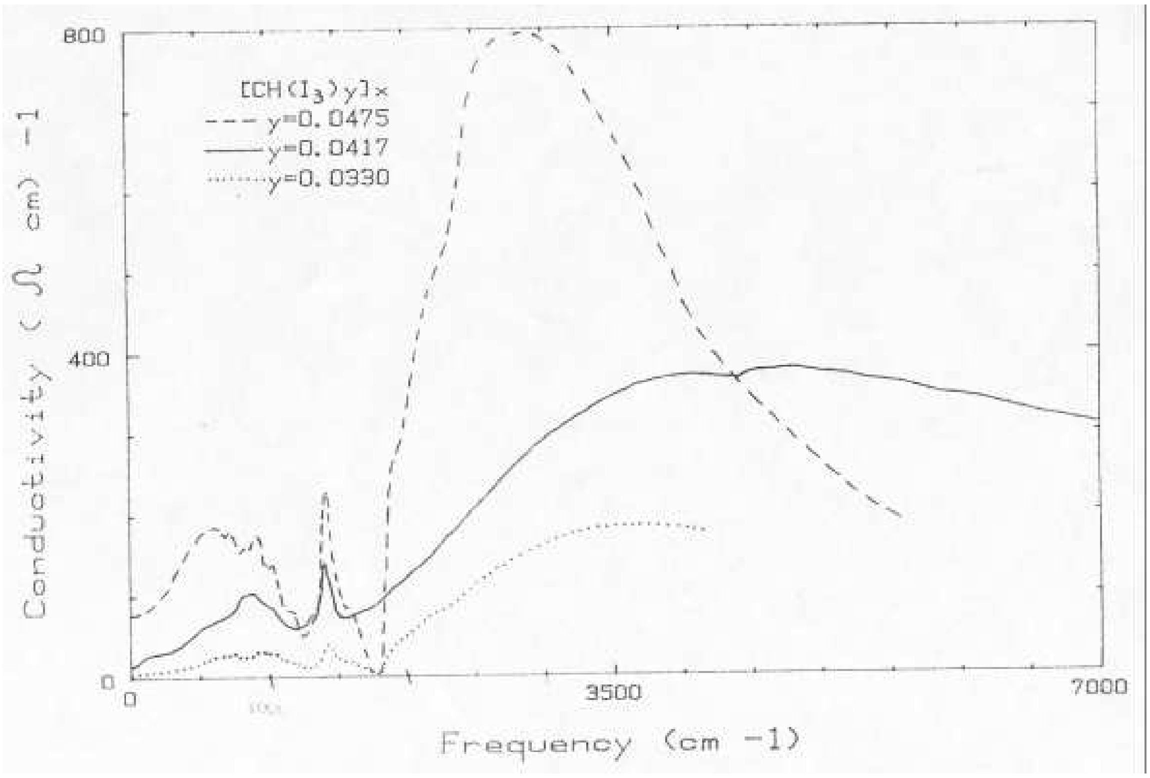

Figure 4: *Cinductivity of heavily iodine doped polyacetylene [3].*

References

[1] F. Wooten, Optical properties of solids

[2] R.J. Bell, Introductory fourier transform spectroscopy.

[3] D.M. Hoffman, Infrared optical properties of polyacetylene.

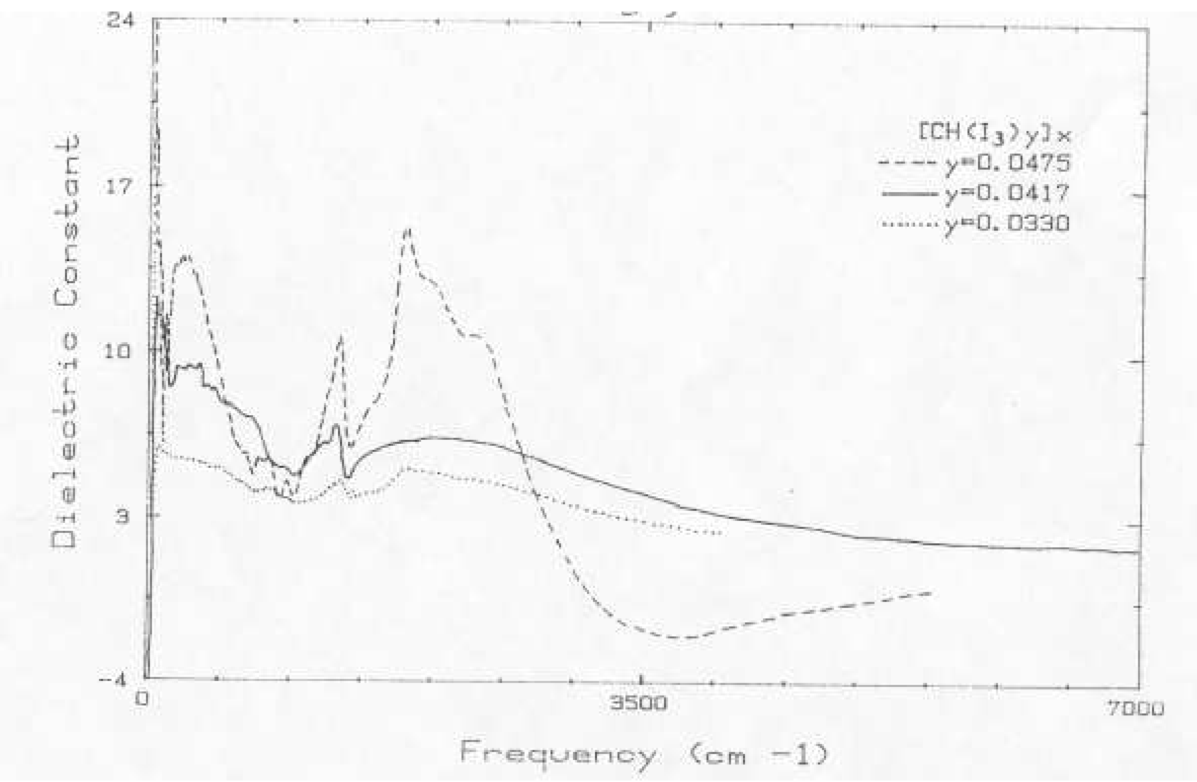

Figure 5: *Dielectric function of heavily iodine doped polyacetylene [3].*