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Modified Drude Model for Terahertz Frequency Range of Conductivity

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ABSTRACT : *The simple Drude model explains well the carrier dynamics for conducting metal. However, the simple Drude model can not explain well for weakly conducting material such as carbon nanotube or conducting polymers. In this research, the simple Drude model is modified by the combination of Cole-Davidson model and localization Drude model. The modified Drude model has low frequency adjustment parameter from localization Drude model and high frequency adjustment parameter from Cole-Davidson model. The modified Drude model fit well to the complex conductivity of aligned carbon nanotube.*

KEY WORDS : terahertz frequency, Drude model, Cole-Davidson model, Localization Drude model, conductivity

1. Introduction

The analysis of conducting material in terahertz (THz) frequency range bases on Drude model which is from Debay theory. The Drude model has been used microwave frequency region or optical region. Some conducting material has big characteristic variations in THz frequency range also it has disagreement between measurement and the Drude model in low and high THz frequency range. Cole-Davidson (C-D) model or Cole-Cole model are introduced to correct the high THz frequency disagreement for doped semiconductor [1][2] and localization Drude (LD) model is also introduced to correct the low THz frequency disagreement for conducting polymer [3][4][5]. Because the characteristic of carbon nanotube has not useful either the C-D mode or LD model, Maxwell-Garnett (M-G) model is used to analysis the characteristic of the material [6][7]. In this research, a new modified Drude (MD) model is introduced using C-D model and LD model. It has less parameters and more simple model compare to M-G model. Because the MD model bases on real part of conductivity of simple Drude model, it requires the Kramer-Krong analysis

2. Analysis of previous Drude model

2.1 Cole-Davidson distribution

The dielectric response for conducting material is described by the following general relationship;

$$\epsilon = \epsilon_{\infty} + i\frac{\sigma}{w\epsilon_o} \qquad (1)$$

where ϵ_∞ is the dielectric constant of intrinsic material, σ is the complex conductivity, and ϵ_o is the free-space permittivity. For the C-D distribution the conductivity is given by [8]

$$\sigma = \frac{\epsilon_o w_p^2 \tau}{(1 - iw\tau)^{\beta}} \qquad (2)$$

where w_p is plasma frequency and τ is the carrier collision time with $\Gamma = 1/\tau$ relation. The C-D distribution corresponds to Drude model with a fractional exponent β limited the values between 0 and 1, and reduce to Drude [9][10][11] model for β=1. Because the Equation (2) is

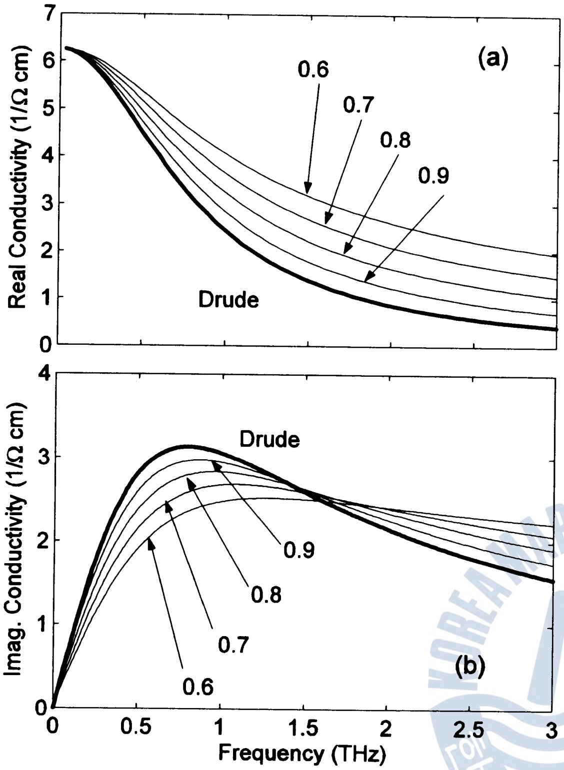

Fig. 1 The Cole-Davidson distribution parameter β is variable from 1 to 0.6. (a) Real part of conductivity. (b) Imaginary part of conductivity.

conductivity, the real and imaginary part of conductivities are directly obtained without using Kramer-Krong analysis. Figure 1 (a) and (b) show the real and imaginary conductivity from β=1 (Drude model) to β=0.6 with $\omega_p/2\pi$ =3THz and $\Gamma/2\pi$=0.8THz. For the small β, the high frequency component of real conductivity increases with the same d.c. conductivity as shown in Fig. 1(a). The imaginary conductivity has decrease at its maximum value with decreasing β as shown in Fig. 1(b). The C-D type complex conductivity accurately described the conductivity of doped silicon [2]

2.2 Localization Drude model

Some conducting polymers have not follow to the simple Drude behavior in real part of conductivity, which has a Lorentzian line shape centered at zero frequency. The characteristic of these materials has small d.c. conductivity

$$\sigma_{LD} = \sigma_{Drude}\{1 - \frac{C/(k_F v_F)^2}{\tau^2} + \sqrt{3w}\frac{C/(k_F v_F)^2}{\tau^{3/2}}\} \quad (3)$$

The LD model is simple Drude model multiplying frequency-dependent real function with a $C/(k_F v_F)^2$ parameter which is not separately determined. Where C is expected to be of the order of unity; k_F is the Fermi wave vector, approximately 10^9 rad/m; and v_F is the Fermi velocity, approximately 10^5 m/s.

Figure 2 shows the simulation of LD model from $C/(k_F v_F)^2$= 1x10^{-26} [s^2] to $C/(k_F v_F)^2$=7x10^{-26} [s^2]. Because Eqn. (3) has only real part of Drude component, the imaginary part of conductivity can be obtained by Kramer-Krong relationship. With increasing $C/(k_F v_F)^2$ parameter, the d.c. conductivity getting smaller and the maximum conductivity moves to the high frequency range. The frequency of crossing point to the curves is 1/3 of damping rate as shown in dashed line in Fig. 2(a). This is always happened to any other values. The imaginary conductivity has also one frequency for each curve's cross

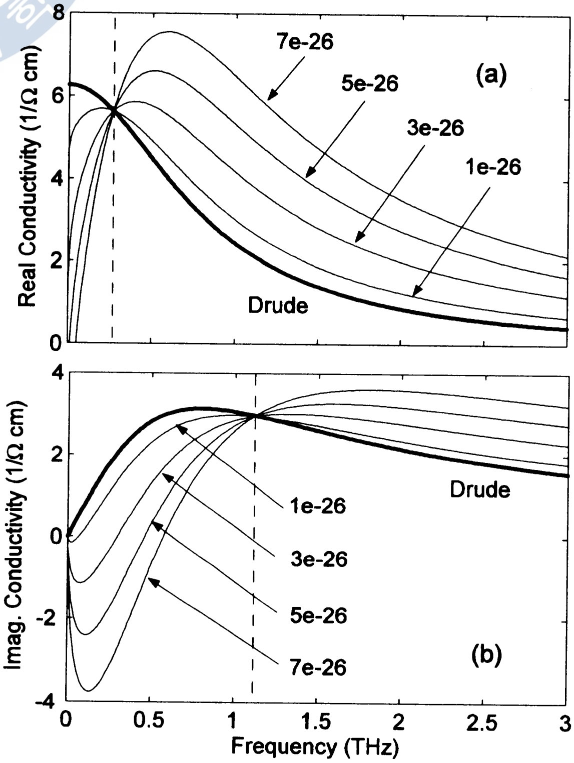

Fig. 2 The localization Drude model for variable $C/(k_F v_F)^2$

point; however, unlike real conductivity, the frequency is around 1.4 times to damping rate.

2.3 Modified Drude model

As shown in Fig. 1(a) and 2(a), the real conductivity can adjust only low and high frequency region. Using these two theory it can be modified one combined model say as MD model given by

$$\sigma_{MD} = \frac{\epsilon_o w_p^2 \tau}{(1 - iw\tau)^3} \{1 - \frac{C/(k_F v_F)^2}{\tau^2} + \sqrt{3w} \frac{C/(k_F v_F)^2}{\tau^{3/2}}\} \quad (4)$$

Figure 3(a,b) and Fig. 4(a,b) show the characteristic curves for the MD model. It follows well C-D and LD characteristic curves. Figure 3 has $\omega_p/2\pi$=3THz, β=0.8, and $C/(k_F v_F)^2$ =7x10^{-26} [s^2] with variable damping rate parameter, $\Gamma/2\pi$, from 0.4THz to 0.8THz. The resonance frequency of real conductivity moves to high frequency region and its magnitude is smaller but the high frequency component goes up as C-D model. Figure 4 has $\Gamma/2\pi$=0.8THz, β=0.8, and $C/(k_F v_F)^2$=7x10^{-26} [s^2] with variable plasma frequency, $\omega_p/2\pi$, from 2.0THz to 4.0THz. Like C-D distribution, d.c. conductivities have same value and the magnitude of each curve gradually increase with increasing plasma frequency. The imaginary conductivity curves are similar compare to imaginary part of LD model as shown in Fig. 2 (b). Using these MD characteristic curves it can be fitted to aligned carbon nanotube film which is not follow C-D distribution and LD model for the measured THz frequency.

The aligned carbon nanotube in Ref [7] has some complex structure which has nanotube network. The carbon nanotube is composed of metallic and semiconducting. The nanotube sample has empty air space created by the network of nanotubes in the sample. Therefore the sample was concerned an effective medium with a carbon nanotube network embedded in an air medium. This carbon nanotube sample did not follow either C-D distribution or LD model. The real conductivity of carbon nanotune follows C-D distribution in high frequency region and follows LD model

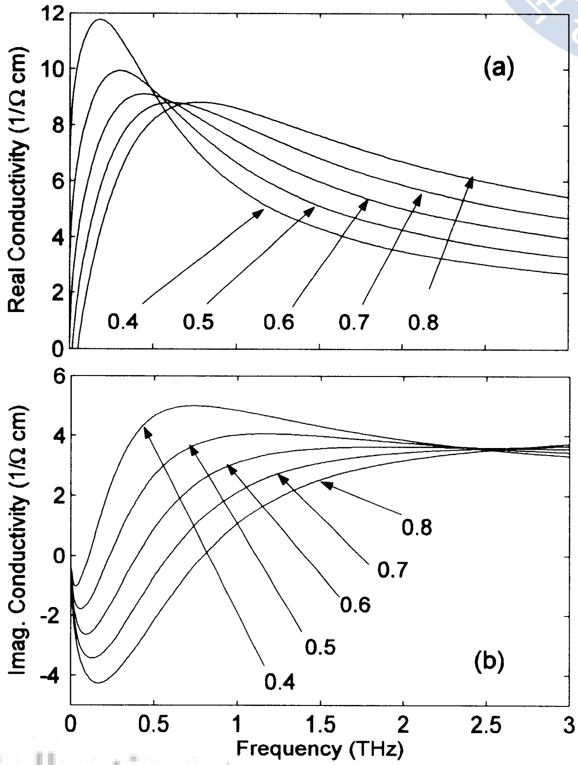

Fig. 3 The modified Drude model for variable damping

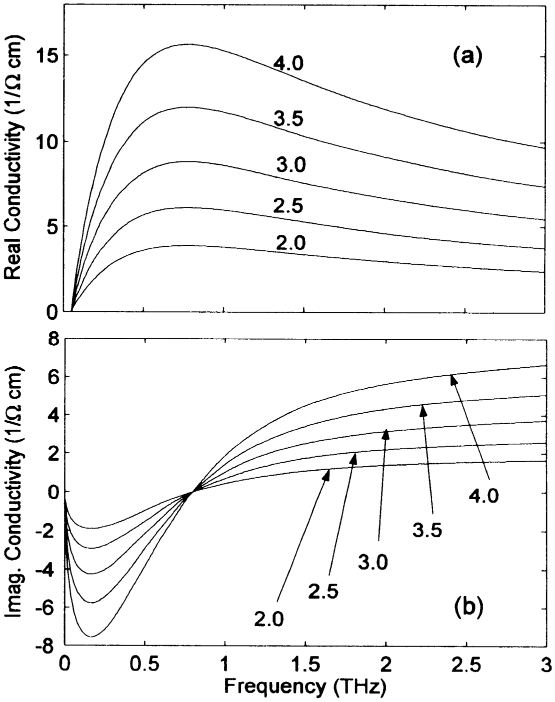

Fig. 4 The modified Drude model for variable plasma

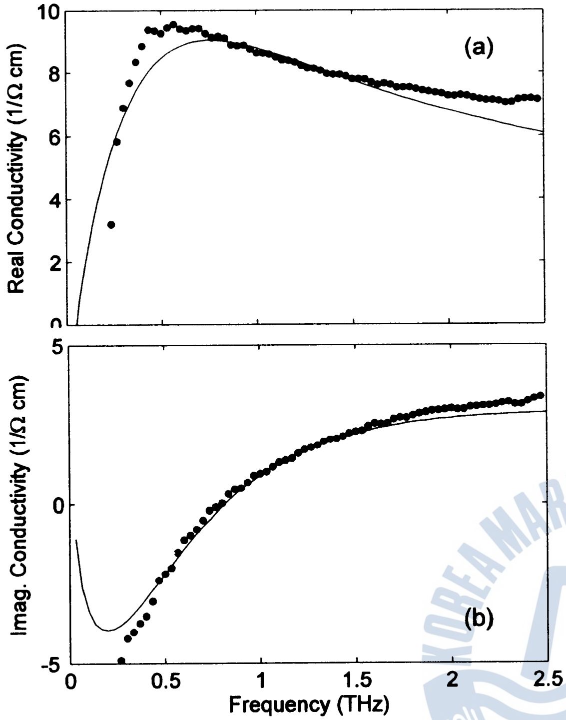

Fig. 5 Comparison of measurement (dots: perpendicularly aligned carbon nanotube) and MD theory (solid line). (a) Real part of conductivity. (b) Imaginary part of conductivity.

in low frequency region.

Figure 5 and 6 show the fitting using MD model to parallel and perpendicular aligned carbon nanotune. The dielectric constant of an effective medium at infinite frequency is 1.8^2 ($\epsilon_\infty=1.8^2$) to get imaginary conductivity. Figure 5 shows perpendicular measurement with MD model using $\omega_p/2\pi=2$THz , $\Gamma/2\pi=0.78$THz, $\beta=0.8$, and $C/(k_F v_F)^2=7.4\mathrm{X}10^{-26}$ [s^2] and Fig. 6 shows parallel measurement with MD model using $\omega_p/2\pi=3.16$THz, $\Gamma/2\pi=0.68$, $\beta=0.8$, and $C/(k_F v_F)^2=9\mathrm{x}10^{-26}$ [s^2]. The measurement in Ref [7] and LD model fit well except high frequency range compare to MG model because these samples have 2.4THz c-direction phonon resonance. The M-G model required seven fitting parameters however, the MD model requires only four parameters. It is more simple compare to M-G model.

carbon nanotube are fit to the MD model expect c-direction phone resonance. As MG model, MD model can adjust low and high frequency values using two known parameters. However, the MD model is more simple compare to M-G model used in previous research.

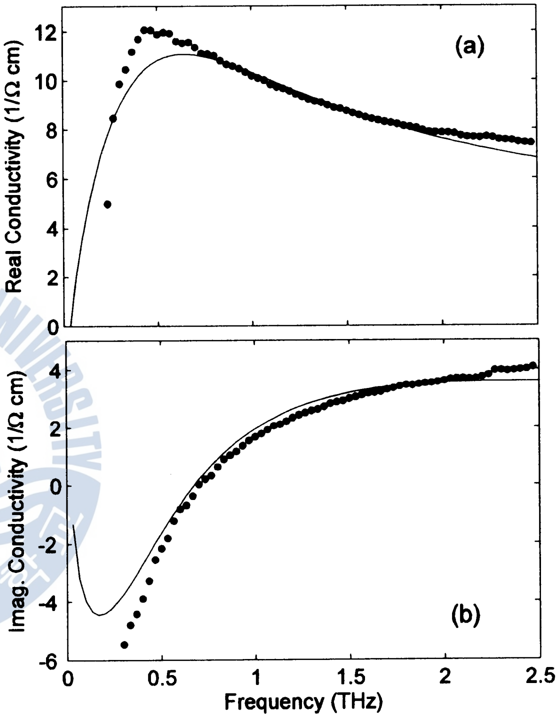

Fig. 6 Comparison of measurement (dots: parallel aligned carbon nanotube) and MD theory (solid line). (a) Real part of conductivity. (b) Imaginary part of conductivity.

Acknowledgments

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