

The Optical Dielectric Model of Cu Thin Film and Its Verification

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Abstract: Cu film was deposited on transparent substrate by magnetron sputtering a Cu target. The Drude-Lorentz optical dielectric model was used to fit the measured reflectance and transmittance data in wavelength range of 300-2200nm. The optical constants, as well as the thickness of the Cu film were obtained. Moreover, the calculated optical constants and the thickness were confirmed by the TFCalc software. It was suggested that the Drude-Lorentz model is suitable for Cu film.

1. Introduction

Copper has been studied over a century because of its extensive applications from metallurgy to semiconductor. Among all the applications, the most attractive use of copper is interconnect. [1] In computer and microelectronics industry, copper plays an important role in the newest development of chip design. Aluminum is being replaced by copper which is used to be the conductor of choice in transistor systems. [2] These applications have increased the requirements for characterizing the physical properties of copper thin film, especially the optical properties related to dielectric constant. It is important during the design of an optical multilayer interference system that the optical constants of all the materials used in it be known. [3] However, with the development of micromation devices, the thickness of interconnect Cu film is reduced to submicron and nanoscale. With the decreases of the thickness, the specific surface area of film increases dramatically, and so the performances of Cu film will be different from copper bulk. Hence, it is necessary and important to determine optical constants of Cu thin film accurately.

In fact, some investigators have devoted to the optical and electrical properties of Cu film. M. Ph. Stoll [4] gave the principle of a polarimetric method for the study of the optical properties of metals, and the method is illustrated with measurements on copper. T. Smith [5] has measured the optical constants of copper and nickel polycrystals at wavelengths 546.1 and 632.8 nm. Ahuja et al. [6] used a non-interacting s-d band model to evaluate $\varepsilon(\omega)$ in copper and calculated $\varepsilon(\omega)$ gave reasonable agreement with measured optical conductivity, where $\varepsilon(\omega)$ is the dielectric function which is bound up with the optical constants. Ya. B. Soskovets et al. [7] have investigated the effect of the structure of smooth copper surfaces on the accuracy of determination of the optical constants of copper. Gong Jun-Bo et al. [8] determined the thickness and optical constants accurately by using newly developed ellipsometry combined with transmittance iteration method in a wavelength range of 300 nm -1000nm, and analyzed the thickness dependence of optical constants of thin oxidized Cu films. M. M. Alam et al. [9] have presented a technique to deposit high strength and highly conductive copper thin films on glass substrates at room temperature.

In this work, Cu film was deposited on transparent substrate by magnetron sputtering a Cu target. Using the measured reflectance and transmittance data, associated with the Drude- Lorentz optical



dielectric model, the optical constants, as well as the thickness of the Cu film were calculated. Moreover the calculated constants were confirmed by the TFCalc software. It was proved that the Drude-Lorentz model is suitable for Cu film.

2. Experimental Details

Cu film was deposited on quartz substrate by sputtering a Cu target (99.99%, purity) with ultra-high vacuum magnetron sputtering system (JGP560B II). The substrate, 0.5mm thick, $2.5\text{cm} \times 2.5\text{cm}$, was cleaned in acetone and ethanol. The target-to-substrate distance was about 6.0cm. Prior to the deposition, the Cu target was pre-sputtered for 5 min to remove surface contaminations. The base vacuum level was $4.0 \times 10^{-4}\text{Pa}$. The flow rate of Ar was 25 sccm and the pressure during deposition was kept at $\sim 0.9\text{ Pa}$. The substrate temperature was 200°C . The deposition time was 10 min, and the sputtering power was 90 W.

The crystal structure of the sample, namely the Cu thin film together with the substrate, was investigated using an X-ray diffractometer (XRD) (MiniFlex II) with Cu K α radiation. The normal incidence transmittance (T) and reflectance (R) of the sample were measured in wavelength range of 300 – 2200 nm by a spectrophotometer (Perkin – Elmer Lambda-950) equipped with an integrating sphere.

3. Results and Discussions

3.1. Crystal Structure of the Sample

XRD pattern of the Cu film was shown in Figure 1. Comparing the results with data from JCPDS international diffraction database, it was found that the peaks at 43.7° and 50.9° correspond to Cu (1 1 1) and Cu (2 0 0), respectively, with (1 1 1) as the preferred orientation. It was the same as our previous results, [9] where the Cu films were deposited on quartz substrates by thermal evaporation.

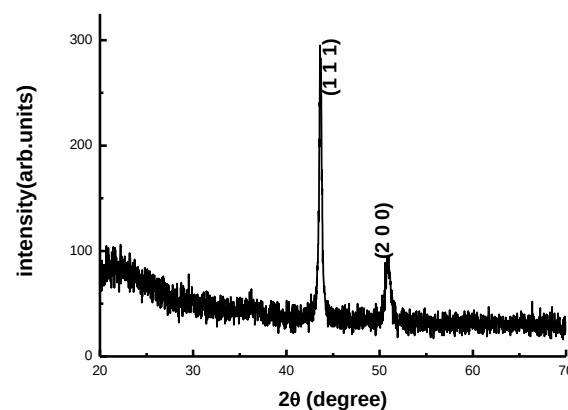


Figure 1. XRD pattern of the Cu film.

Also, it was consistent with the results reported by other authors, [1,2] and must be attributed to the energy of the Cu particles hitting on the surface of the substrates.[10]

3.2. Optical Constants and Thickness of the Cu Thin Film

Commonly, the optical constants are retrieved by simulating the transmittance and (or) reflectance based on dielectric models and by using a nonlinear least squares fitting procedure. [11] The as-deposited Cu film is a metal film. Accordingly, the Drude - Lorentz model was used to determine the optical constants of the Cu film from the reflectance and transmittance data, which combines the Drude model with the Lorentzian oscillator model and has been applied in metal film by Baron et al.

[12] The dielectric function of the Drude - Lorentz model can be expressed as [13]

$$\varepsilon(\omega) = \varepsilon_1 + i\varepsilon_2 = (n + ik)^2 = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\omega_0^2}{\omega_0^2 - \omega^2 + i\Gamma\omega\omega_0} - \frac{\omega_D^2}{\omega^2 - i\omega_\tau\omega} \quad (1)$$

Where ε_∞ and ε_s represent the high- and low-frequency dielectric constants, respectively. Accordingly, ω_0 is oscillator resonance frequency, Γ is the damping factor of the oscillator, ω_D is the plasma resonance frequency, ω_τ is the collision frequency, and ω is the angular frequency of incidence wave.

Based on the optical dielectric function in Eq. (1), a computer program was written in FORTRAN for calculating the refractive index (n), extinction coefficient (k), and its thickness (d) of the Cu film by simulating the reflectance and transmittance data. A merit function f was defined as

$$f(d, n(\lambda), k(\lambda)) = \sum_{\lambda} [T_{meas}(\lambda) - T_{calc}(\lambda)]^2 + \sum_{\lambda} [R_{meas}(\lambda) - R_{calc}(\lambda)]^2 \quad (2)$$

Where λ was wavelength, $T_{meas}(\lambda)$ and $R_{meas}(\lambda)$ referred to the measured transmittance and reflectance, respectively. $T_{calc}(\lambda)$ and $R_{calc}(\lambda)$ referred to the calculated transmittance and reflectance, respectively. In the calculation process, d and the parameters of dielectric function were adjusted so that the calculated spectrum was close to the measured spectrum to full extent and the merit function had the minimum.

Figure 2 showed the measured and calculated transmittance and reflectance of the sample. It could be seen that the calculated transmittance and reflectance were in good agreement with the measured ones.

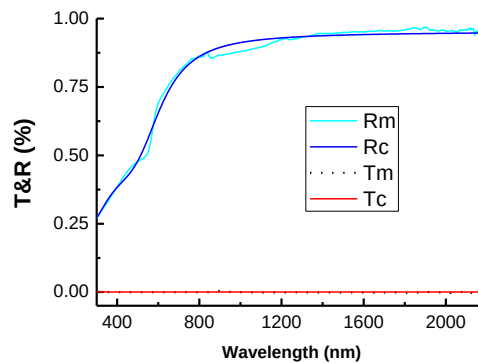


Figure 2. The measured and calculated transmittance and reflectance of the sample.

Based on the measured data in Figure 2, optical constants n and k and the thickness d of the Cu film can be obtained by using eqs. (1) and (2), and a computer program. Figures 3 (a) and (b) displayed the calculated refractive index and extinction coefficient of the Cu film, respectively. The calculated results indicated that d of the Cu thin film was 123 nm. The optical constants of Cu thin film obtained from handbook [14] were also presented in Figures 3. It was found that the relationships of both the refractive index and the extinction coefficient with the wavelength were similar to the ones from handbook, respectively. Both n and k increase with an increase in wavelength in the infrared region, due to Cu being a good conductor. [15] On the other hand, it was evident that our refractive indexes were larger than those from handbook. This must be attributed to sputtering technique. The film used in the handbook was obtained by evaporating. So the density of our film was large than that of handbook, resulting in the increase of refractive index.

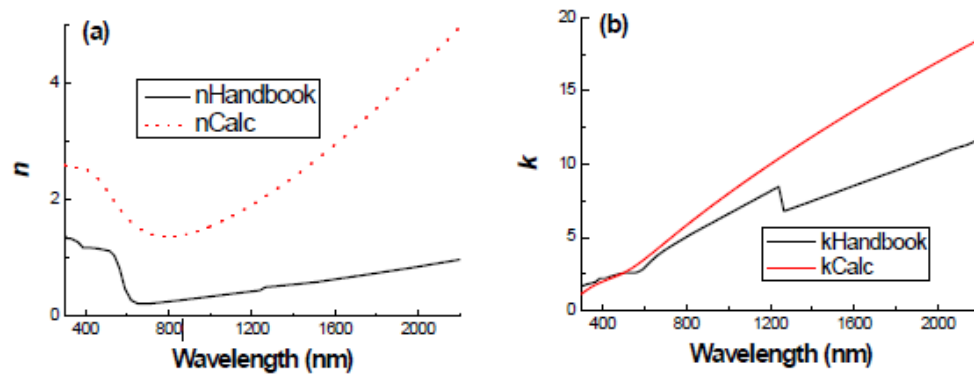


Figure 3. The calculated (a) refractive index and (b) extinction coefficient of the Cu film and the ones obtained from handbook.

3.3. Verifying the Optical Dielectric Model

TFCalc is one of the most commonly used tools for the design and analysis of optical thin film. Put the optical constants both of quartz and Cu thin film calculated in Sec. 3.2, as well as its calculated thickness, into the TFCalc software, the reflectance (R_{Tfc}) and transmittance (T_{Tfc}) of sample were obtained once again. Due to the transmittance went near to zero, only the measured reflectance and the one calculated from TFCalc were shown in Figure 4.

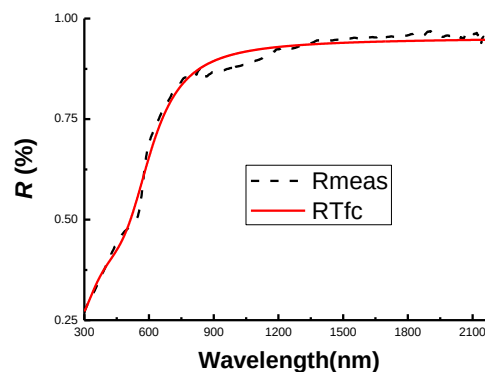


Figure 4. The measured reflectance and the one coming from TFCalc.

It could be seen from Figure 4, the reflectance resulting from TFCalc was in good agreement with the measured one in all over the wavelength range of 300 – 2200 nm. So, it could be received definitely that the Drude - Lorentz model was suitable for the Cu thin film. Moreover, it was comprehensible. The Drude - Lorentz model basically made of the contributions of the high frequency lattice dielectric constant, ϵ_∞ , which represents the contribution to $\epsilon(\omega)$ outside of the simulated range, the Lorentz oscillator, i.e. the second term of the complex dielectric function, which describes the behavior of the dispersion law in the near UV spectral region and characterizes the dielectric properties of Cu thin film, determines the variation of the optical band-gap energy, and the Drude oscillator, i.e. the third term of the complex dielectric function describes the free-carriers in the near-IR spectra and, as a consequence, the conductive properties of the Cu films. In fact, the Drude - Lorentz model, namely eq. (1), is one of the oldest but the most used classical dispersion law [16] and has also been applied to investigate the optical properties of indium tin oxide (ITO) thin films. [17]

4. Conclusions

Cu film was deposited on transparent substrate by magnetron sputtering a Cu target. The crystal structure of the sample was investigated using an X-ray diffractometer (XRD) (MiniFlex II) with Cu K α radiation. The normal incidence transmittance (T) and reflectance (R) of the sample were measured in wavelength range of 300-2200 nm by a spectrophotometer (Perkin – Elmer Lambda-950) equipped with an integrating sphere. Using the measured reflectance and transmittance data, associated with the Drude- Lorentz optical dielectric model, the optical constants, as well as the thickness of the Cu film were calculated. Moreover the calculated constants were confirmed by the TFCalc software. It was proved that the Drude-Lorentz model is suitable for Cu film.

5. Acknowledgements

This work was financially supported by the Natural Science Foundation of Fujian Province of China (2014J01016).

6. References

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