Phase shift and penetration depth of metal mirrors in a microcavity structure

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Optical properties of metal films, such as phase shift on reflection or penetration depth of electromagnetic waves into mirrors, play an important role in determining the resonance wavelength of a microcavity. We created a series of $\lambda/2$ cavities with a symmetrical structure of glass/Ag/lithium fluoride/Ag by changing the thickness of the Ag film. The penetration depth at different thicknesses of Ag film was obtained from the transmittance peaks of the cavities. Phase shift on reflection at the lithium fluoride–Ag interface was calculated based on the measured optical constants. The formulation between phase shift and penetration depth was proved by experimental results, which are in good agreement with the theoretical calculations.

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1. Introduction

An optical microcavity is a resonator that has at least one dimension of the order of a single optical wavelength [1]. When inserting emitting materials into a microcavity, optical emission properties of materials, such as spontaneous emission rate, emission color, and spatial distribution of radiation power, can be significantly modified [2–5]. The ability to control the spontaneous emission of an emitter has many practical applications in various optoelectronic devices such as light-emitting diodes (LEDs) and lasers based on inorganic or organic semiconductor materials [5–8].

Metal mirrors are frequently used in microcavities since they can provide suitable reflectance and excellent electrical contact. According to electromagnetic theory, part of the energy of incident electromagnetic waves from a dielectric material is absorbed by the metal. So unlike the case at the interface between two dielectrics, the phase shift on reflection at a dielectric–metal interface is neither 0 nor π. This phase shift can also be interpreted as the penetration depth of electromagnetic waves into metal mirrors. Thus the effective cavity length of a microcavity is given by the sum of the optical thickness of cavity layers and mirror penetration depths. So the phase shift that accompanies reflection from the metal–dielectric interface is of great importance when metals are used in microcavities. Determination of the resonance wavelength λ of a microcavity for normal incidence is generally expressed by the following Fabry–Perot equation:

$$2\left(\sum_i n_i d_i + L_{\text{pen1}} + L_{\text{pen2}}\right) = m\lambda, \tag{1}$$

where the first term of Eq. (1) defines the optical thickness of cavity layers between two mirrors, n_i and d_i are the refractive index and thickness of the cavity layers, L_{pen1} and L_{pen2} are penetration depths of the respective mirrors, and m is the mode index. When applying to a normal microcavity organic LED, which has a basic structure of two parallel mirrors (distributed Bragg reflector and metal mirror), the penetration depth in a metal mirror is always neglected because it is small compared with the whole cavity length. However, in most cases it should not be neglected, especially when a cavity length is of the order

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of an optical wavelength, otherwise the resonance wavelength of a microcavity device may have an error of a few tens of nanometers. Therefore, for proper design of an optical microcavity, precise determination of the phase shift and the penetration depth of a metal is of great importance.

Although the electromagnetic theory associated with the phase shift on reflection is simple, sign convention for the phase factor of electromagnetic sinusoidal waves is frequently overlooked or not stated clearly, which will result in quite different phase shift amplitudes. Inconsistency was found not only in the expression of the phase shift, but also in that of the relation of the phase shift (β) and the penetration depth (L_{pen}). Although $L_{pen} = \lambda\beta/4\pi$ was reported by most authors [9–11], the following equation:

$$L_{pen} = \frac{\lambda(\pi - \beta)}{4\pi}, \tag{2}$$

was also reported [12,13]. Apparently the penetration depth based on $\lambda\beta/4\pi$ and Eq. (2) are significantly different.

To obtain the correct relation between phase shift on reflection and penetration depth of a metal mirror, microcavities with the structure of air/Ag/lithium fluoride(LiF)/Ag/glass were investigated. LiF is employed because it has well-defined optical properties in the visible spectral region. Microcavities are constructed to have an optical thickness of $\lambda/2$ and equally thick metal mirrors. It is convenient to determine the penetration depth of a metal mirror by selection of a $\lambda/2$ cavity.

We report the results of the phase shift and penetration depth of metal mirrors in microcavities. Good agreement between the theoretical and the experimental results shows that Eq. (2) is the proper expression for the relation of penetration depth and phase shift.

2. Experimental

The Ag mirrors and the LiF films were deposited by electron beam evaporation under 5×10^{-4} Pa. Ag films were deposited at the rate of 1 nm s^{-1}. LiF films were deposited at the rate of 0.3 nm s^{-1}. The thickness of all the films was monitored by a crystal oscillator during deposition, and the actual thickness was calibrated by an atomic force microscope. The optical constants of Ag and LiF were measured with the UVISEL spectroscopic phase-modulated ellipsometer (Horiba Jobin Yuon, Beijing, China). Transmittance spectra were measured with an ultraviolet–visible–near-infrared scanning spectrophotometer, UV-3101PC, manufactured by Shimadzu, Kyoto, Japan.

3. Results and Discussion

Optical constants of LiF (measured at a thickness of 210 nm) and Ag (at the thickness of 50 nm) are shown in Fig. 1. LiF shows no absorption in the visible spectral region and has a refractive index of 1.52 at 400 nm wavelength. The refractive index of LiF decreases with wavelength. The refractive index of Ag is 0.119 at a wavelength of 400 nm, which changes little with wavelength. Ag has a big k value of 1.944 at 400 nm that increases with wavelength.

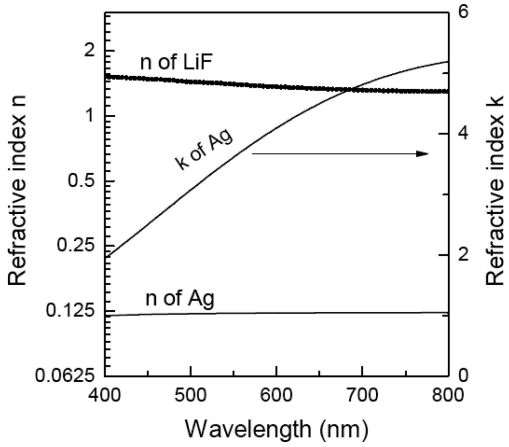

Fig. 1. Optical constants of LiF and Ag.

The definition of phase shift on reflection at the interface between a dielectric and a metal is shown in Fig. 2. Here the sign convention for the phase factor of electromagnetic sinusoidal waves is $\exp[i(\omega t - \mathbf{k}\cdot\mathbf{r})]$, which is the more conventional version in thin-film literature. The amplitude and phase of the reflection coefficient can be calculated from the optical constants of the metal and dielectric films. Assuming that the incident medium has a refractive index of n_0, the metal film has a complex refractive index of $n_1 - ik_1$, where n_1 is the refractive index and k_1 is the extinction coefficient. Then the Fresnel amplitude reflection coefficient for the metal film can be written as

$$r = \frac{E_r}{E_i} = |r|e^{-i\beta} = \frac{n_0 - (n_1 - ik_1)}{n_0 + (n_1 - ik_1)} = \mathrm{Re}(r) + i\mathrm{Im}(r), \tag{3}$$

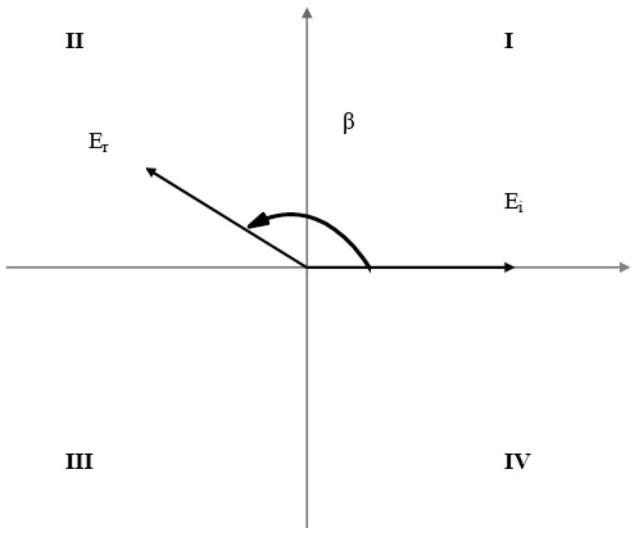

Fig. 2. Definition of phase shift β.

where E_r and E_i are the complex amplitudes of the electric fields of reflected and incident electromagnetic waves, respectively, and $|r|$ is the modulus of r. Thus, phase shift β is the angular difference between E_r and E_i. Im(r) and Re(r) are the imaginary part and the real part of the reflection coefficient. When light is incident through the dielectric on a bulk metal or a thick metal film, the phase shift on reflection is given by

$$\beta = \arctan \frac{\mathrm{Im}(r)}{\mathrm{Re}(r)} = \arctan \frac{2n_0k_1}{{n_0}^2 - {n_1}^2 - {k_1}^2}, \quad (4)$$

In agreement with what Bennett reported [14], this phase shift is defined as the absolute phase shift. Because metal has a big k value, $\mathrm{Im}(r) > 0$ and $\mathrm{Re}(r) < 0$. Phase shift β lies in the second quadrant, as shown in Fig. 2. It should be noted that β would lie in the third quadrant if the phase factor of $\exp[i(\mathbf{k} \cdot \mathbf{r} - \omega t)]$ were used [13,15].

The reflection phase shift changes with thickness. In the case of a thin metal film, the Fresnel amplitude reflection coefficient has a more complicated form that is due to the effect of multibeam interference. Here, we use the transfer matrix method to simulate the metal phase shift, the transmittance spectra, and the standing wave electric field distribution of microcavity structures. Figure 3 shows the dependence of the reflection phase shift of Ag on wavelength and thickness. The phase shift is calculated by the measured optical constants of LiF and Ag given in Fig. 1. Figure 3 shows that the phase shift on reflection is 1.813 at a thickness of 50 nm and wavelength of 400 nm, and decreases with film thickness and increases with wavelength over the visible range.

As shown in Fig. 4, confined electric field amplitude as a function of position along the cavity axis was given for the following two microcavities:

microcavity(a): air/ideal metal(50 nm)/LiF(174 nm)/ideal metal (50 nm)/glass;

microcavity(b): air/Ag(50 nm)/LiF(125 nm)/Ag(50 nm)/glass.

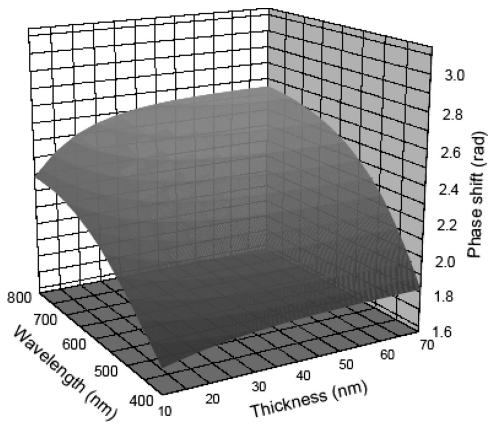

Fig. 3. Dependence of the phase shift of metal Ag film on thickness and wavelength.

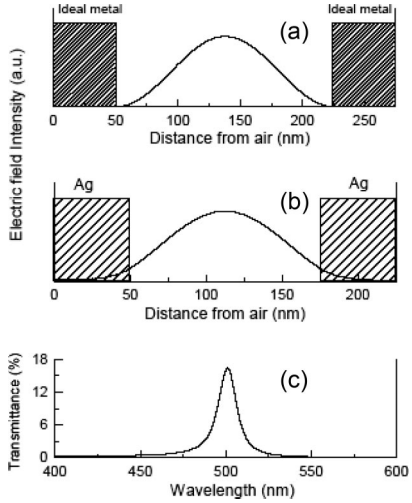

Fig. 4. Comparison of electrical field distribution in the (a) ideal and (b) real metal microcavities. (c) The measured transmittance spectrum of microcavity (b).

The metal in microcavity (a) is treated as a perfect conductor, and no electric field can penetrate into it. There is a node exactly at the metal–dielectric interface, where reflection takes place, and there is a response of π out of phase with respect to the electric field incident upon it. In this case the phase shift at the interface is π and the penetration depth is zero. The LiF film, with a thickness of 174 nm, determines the cavity length of 250.4 nm and resonance wavelength of 501 nm. For the real metal material of Ag in microcavity (b), the phase shift on reflection is no longer π. The reflection does not take place at the interface, and the node is behind the metal. The penetration depth into the metal film from the dielectric medium can be designated as the distance between the location of the nearest node inside the metal and the metal–dielectric interface, which can be written in the form of Eq. (2). It is well known that the peak of the transmittance spectrum of a microcavity corresponds to the resonance wavelength of the microcavity, the knowledge of which can be used to predict the effective cavity length. Figure 4(c) shows the measured transmittance spectrum of microcavity (b) and also shows that the 125 nm thick LiF film results in a resonance wavelength of 501 nm because of the effect of the penetration depth of a Ag mirror. This resonance wavelength is in good agreement with our simulated results obtained by use of Eq. (2).

To validate Eq. (2) further, we created a series of cavities. The same 125 nm thick LiF film was used for all the devices, but the thickness of Ag was varied from 10 to 50 nm. As a result, the resonance peaks changed accordingly. Figure 5 shows the resonance peaks as well as the mirror penetration depths at different thicknesses of Ag. Curves (a) and (b) in Fig. 5 represent the simulated penetration depths of the Ag film at the glass side and the air side, respectively, showing that the penetration depth of the Ag film at the two sides has a slightly larger difference when the Ag film is thinner. The difference can be neglected

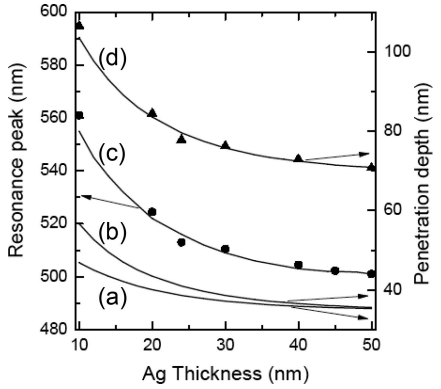

Fig. 5. Dependence of penetration depth and resonance wavelength on Ag thickness. Curve a, simulated penetration depth of the metal Ag mirror at the glass side; curve b, simulated penetration depth of the metal Ag mirror at the air side. Curve d, sum of the simulated penetration depth of the two metal Ag mirrors. The filled triangles represent the sum of the experimentally determined penetration depth. Curve c, simulated resonance wavelength of the microcavities. The filled circles represent the resonance wavelength obtained by experiment.

when the Ag film is thicker than 40 nm. The difference is approximately 10 nm when the Ag film is 10 nm thick because, when the Ag film is thinner, the effect of multibeam interference on reflection must be taken into account. The complete reflection coefficient is determined by the thickness and the reflection coefficients at the two interfaces of Ag when considering the multibeam interference. So the difference in reflection coefficients between the Ag–air interface and the Ag–glass interface results in different penetration depths in curves (a) and (b) in Fig. 5. Curve (c) in Fig. 5 shows the simulated (solid curve) and experimental (filled circles) resonance wavelengths for transmission as a function of the Ag thickness. The simulated results tallied basically with the experimental ones within the range of the admittance error. The discrepancy of 6 nm between the simulated transmittance peak (555 nm) and the experimental one (561 nm) was found when the Ag film was 10 nm thick. This can be explained as follows: during the calculation it was assumed that the optical constants of Ag did not vary with the thickness and the films were continuous and uniform, but the optical constants of a thin Ag film might differ from those of the thick film. Curve (d) shows the simulated penetration depths [the sum of curves (a) and (b), solid curve] and the experimental ones (filled triangles), which were obtained from the experimental transmittance peaks (filled circles) by subtraction of the optical thickness of LiF from the effective cavity lengths. Good agreement of the penetration depths from two different methods shows that Eq. (2) is the proper form for the relation of phase shift and penetration depth.

4. Conclusions

In conclusion, we have shown that the phase shift on reflection plays an important role in determining the resonance wavelength of a microcavity. To clarify the expressions between the penetration depth and the phase shift on reflection at a metal–dielectric interface, we designed and fabricated a series of cavities with a structure of glass/Ag/LiF/Ag by changing the thickness of Ag film and maintaining a LiF thickness of 125 nm. By comparing the simulated penetration depths and the experimental ones the proper relation of phase shift and penetration depth is proved.

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