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A Multi-layer Film Model for Formation Mechanism of Bright Whiteness in Beetle Scale

Xiaoping Li and Zirong Tang
Wuhan National Laboratory for Optoelectronics
Huazhong University of Science and Technology,
Wuhan, China 430074
{lixp & zirong}@mail.hust.edu.cn

Rizwan Malik, Tielin Shi, Wuxing Lai and Shiyuan Liu
State Key Laboratory of Digital Manufacturing Equipment and Technology
Huazhong University of Science and Technology
Wuhan, China 430074
rizwanmali@yahoo.cn

***Abstract* - By taking the optical imaging of the internal micro-nanostructure of white beetle scales, a multilayer aperiodic model is presented in this paper to understand the complex natural formation mechanism of bright whiteness of a kind of white color beetle. Based on the proposed model, optical simulations of visible light reflectivity are conducted correlated with the variation of layer number, layer thickness and incident angle of visible light with alteration of the air-layer and chitin layer. The results showed larger incident angle will lead to lower reflectivity, smaller number of layers will also lead to lower reflectivity and higher fluctuations within the range of visible bandwidth. The simulated results match well with the measured reflective data, and the proposed model is reliable to interpret the formation mechanism of bright whiteness in beetle scale. The work here is an effect to further fabricate novel high-brightness optical composite films or coating materials for a variety of applications.**

Index Terms* - *multi-layer film; structure color; whiteness; model.

I. INTRODUCTION

Structural color in nature, which has a pure physical origin such as diffraction or interference of light, has long been a problem of scientific interest. It has attracted great interest recently because of its envisioned applications in many emerging fields, including bio-inspired advanced materials such as paint, cosmetics, textiles and etc.[1]. As the research progresses, it has become clear that most the structure colors originate from basic optical processes represented by thin-film interference, multilayer interference, diffraction-grating effect, photonic crystals, light-scattering and so on [2-5]. Beetles have become a prominent focus of spreading various colors in nature, as shown in Fig. 1(A), Whiteness is relatively rare in animals and among them, white color beetle "Cyphochilus" has developed scales that effectively reflects all visible wavelengths of light in order to appear white, which also presents more distinctive bright whiteness phenomena that investigate encouragement for the scientists [6-9]. Its white color helps the insect better camouflage among white fungi found in its native habitat and, as shown in Fig. 1(B), which is rarely studied and may have implications for novel biomimetic white materials. The whiteness of the beetle scale is recently assumed to be the result of multiwavelength scattering arising from aperiodic and multiply oriented interfaces between low-absorbance media of appropriately different refractive index, which originates from elongated flat white scales that imbricate its body.

These scales are reported to be about 5 micron thick, 250 micron long and 100 micron wide, as shown in Fig. 1(C). In the meanwhile, optical measurement of bright whiteness for beetle scale is also reported that it is even brighter than milk teeth with overall reflectance of closing to 70% in visible bandwidth, and the reason of high reflectance of white beetle scale is assumed due to its special orientation of chitins inside the scale structure [10].

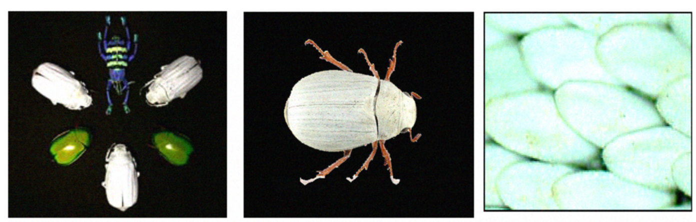
(A) (B) (C)

Fig.1 (A) Colorful beetles, (B) White beetle, (C) Scale of white beetle

If we view synthetically into the chitin layer then we will find that it has following structure as shown in Fig .2 [11].

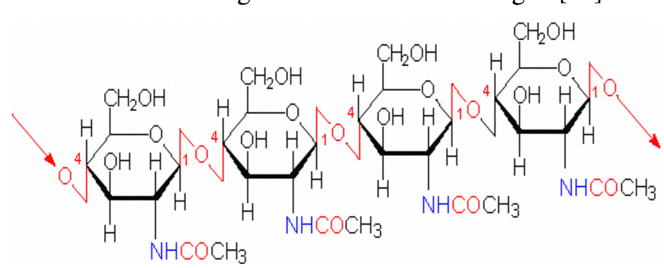

Fig. 2 Chemical structure of Chitin layer in Cyphochilus beetle

Actually structure shows that there are covalent bonds between $NHCOCH_3$, H_2O and CH_2OH that cause the clear reflection back to the source and into the atmosphere with

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respect to the surface light reflection law “Fresnel’s Law”, according to which if the incident light beam is white then the light reflected from the surface will also be white. As there is very strong bonding in chitin layer, therefore, light can not diffuse permanently towards the bottom layer but 0.35 % of light part diffuses at the first time of incidence that is considered negligible in further analyzation process.

However, the real mechanism of whiteness formation in beetle is not clear up to now. Since whiteness can be originated from quite a few mechanisms [12-14]. This paper will propose a whiteness formation mechanism based on a multi-layer aperiodic film interference model. The beetle scale is treated as multi-layer films with alteration of the air-layer and chitin layer, then reflectivity of the structure is simulated with optical analysis, and simulation results are compared with the experimental data to verify the model.

II. Modeling and Simulation

The internal micro-nanostructures of the white beetle scales were reported previously, as shown in Fig. 3. Fig. 3(A), (B) and (C) are scale arrangement, SEM image and TEM image of crossection, respectively. As shown in Fig. 3(C), the interiors of the scale are composed of network of interconnecting cuticular filaments or chitin, which can be regarded as layer-by-layer chitin and air, although each layer of chitin consists of random distribution of filaments. Therefore, the work here will treat the scale cross-section as layer-by-layer thin film structure with alteration the layer material by air and chitin, in the meantime, the air-layer thickness or depth will be treated as randomly to match with optical imaging of scale cross-section as shown in the structure.

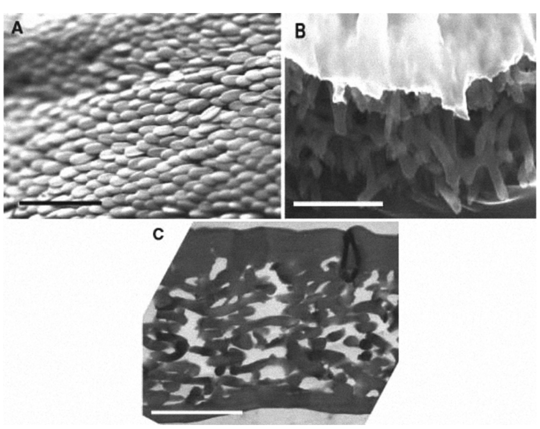

Fig. 3 （A）Cyphochilus beetle scale, （B）cross-section SEM of beetle scale, （C）TEM of the section [Courtesy from P. Vukusic, etc. Science, 315(2007)348]

Therefore, the controlling parameters of multi-layer film physical model will be the layer number, layer thickness and the refractive index of chitin, as shown in Fig. 4. Except the top and bottom layer, where the thickness is fixed, inside layers with alteration of chitin and air layer will vary to optimize the design. On the other hand, the incident light angle within the visible bandwidth from 400 to 700nm is another controlling parameter for optical modeling and simulation.

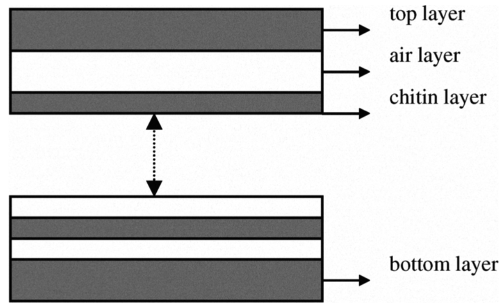

Fig. 4 Schematics of physical model for the multi-layer aperiodic films

Conventional calculations of optical properties for multilayer films are based on Maxwell equations and boundary conditions, which is very complicated and time-consuming for calculations. In this work, a special matrix approach is presented. For a K-layer film system, such as shown in Fig. 5,

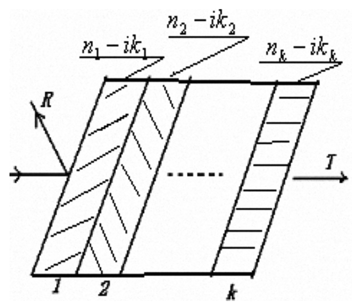

Fig. 5 Schematic of the multi-layer system.

Each layer of the matrix can be expressed as:

$$\begin{bmatrix} \cos\delta_j & i\sin\delta_j/\eta_j \\ i\sin\delta_j\eta_j & \cos\delta_j \end{bmatrix} \quad (1)$$

Where every parameter of film is included,

$\delta_j = \frac{2\pi}{\lambda} N_j d_j \cos\theta_j$

and $\eta_j = n_j - iK_j$

For each layer using same boundary condition, as the following,

$$\begin{bmatrix} B \\ C \end{bmatrix} = \left\{ \prod_{j=1}^{k} \begin{bmatrix} con\delta_j & i\sin\delta_j/\eta_j \\ i\sin\delta_j & con\delta_j \end{bmatrix} \right\} \begin{bmatrix} 1 \\ \eta_s \end{bmatrix} \quad (2)$$

Where refractive angle is defined by the rule

$$n_0 \sin\theta_0 = (n_j - iK_j)\sin\theta_0 \quad (3)$$

Reflectivity of the film system can be calculated as

$$R = rr^* = \frac{|\eta_0 - Y|^2}{|\eta_0 + Y|^2} = \frac{|\eta_0 B - C|^2}{|\eta_0 B + C|^2} \qquad (4)$$

Transmittance of the film system can be calculated as

$$T = \frac{\eta_s}{\eta_0} tt^* = \frac{4\eta_0 \eta_s}{|\eta_0 B + C|^2} \qquad (5)$$

Therefore each parameter of the each film layer can be obtained for calculation of refractivity of film system.

Based the proposed physical model, simulations are conducted by commercial software Essential Macleod with a well-defined algorithm for optical simulation. Fig. 6 is the algorithm for the optical simulation process with the model. The whole algorithm is described as following. First input air-layer, chitin layer and incident light parameters such as layer thickness, refractive index, layer number, light angle, wavelength and range of wavelength, then through thin-film interference theory to calculate the reflectivity of light for each wavelength, and compare the calculated results with set-value to optimize the input data such as layer number and thickness or depth, repeat the process until an optimized result is obtained. Therefore, with the defined value of input parameters while varying the air-layer thickness and layer number, through so-called needle optimization, the reflective light interference results of incident light can be obtained and the design of multi-layer film can be optimized.

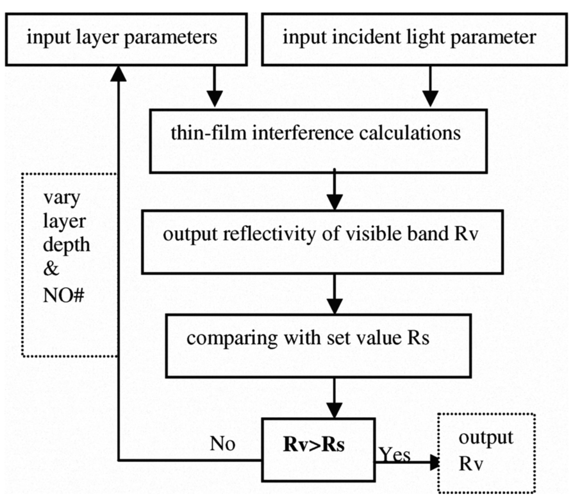

Fig. 6 Algorithm of the optical simulation process

III. Results and Discussions

As the refractive index plays an important role in understanding light reflection phenomena, it is very critical for determination of refractive index for different layers. In this work, the refractive index of chitin layer in this model is assumed to be around 1.58 having the layer thickness of 250nm except the top and bottom layer thickness. During simulation, the layer number varies from 15 to 41 while overall thickness of scale variation varies from 3 to 5 micron. For better understanding the whiteness formation, the incident light angle is also considered in this work.

For different incident angle of 0, 10 and 20 degree with respect to the vertical direction. Through simulation, the effects of incident angle and layer number on reflectivity can be obtained. Fig. 7 to 9 shows the simulated results for layer number of 41, 31 and 21 respectively.

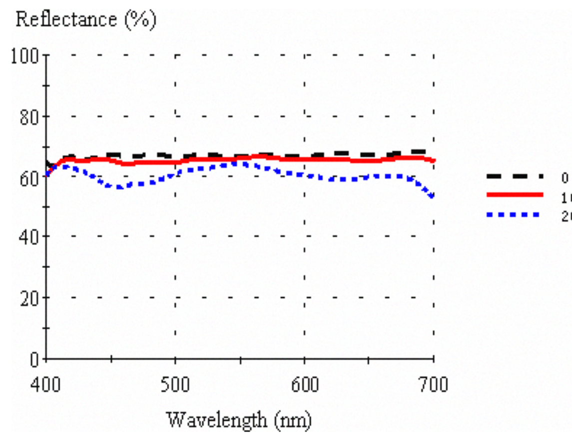

Fig. 7 Reflectance vs wavelength at layer number of 41 and incident angle of 0, 10 and 20 degree, respectively.

As shown in Fig. 7, which simulates the layer number of 41 for reflectance with respect to visible light wavelength, the highest reflectance of around 68% is obtained for 0 degree of incident angle. When the incident angle reaches 20 degree, the large variation of reflectance is observed with the visible light wavelength, and the reflectance variation ranges from 50% to 65%.

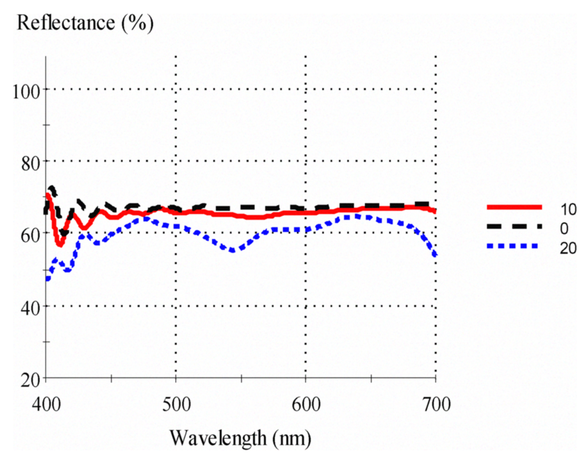

Fig. 8 Reflectance vs wavelength at layer number of 31 and incident angle of 0, 10 and 20 degree, respectively.

As shown in Fig. 8, which simulates the layer number of 31 for reflectance with respect to visible light wavelength, the highest reflectance of around 65% is obtained for 0 degree of incident angle; however, there is a large fluctuation at the lower wavelength approaching 400nm. When the incident angle reaches 20 degree, the even larger variation of reflectance is observed at both ends of visible light wavelength (around 400nm and 700nm).

As shown in Fig. 9, which simulates the layer number of 21 for reflectance with respect to visible light wavelength, the highest reflectance of around 63% is obtained for 0 degree of incident angle. Again, there is a large fluctuation at the lower wavelength approaching 400nm. When the incident angle reaches 20 degree, the even larger variation of reflectance is observed at both ends of visible light wavelength (around 400nm and 700nm).

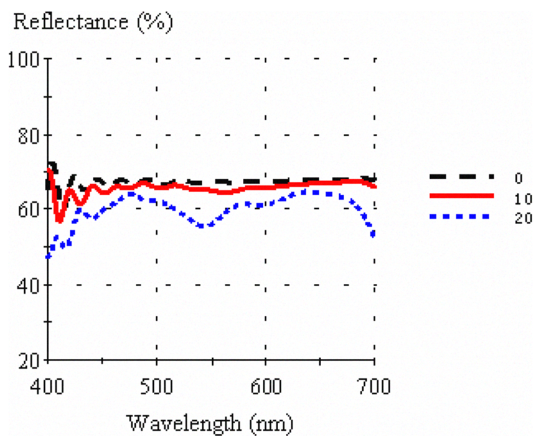

Fig. 9 Reflectance vs wavelength at layer number of 21 and incident angle of 0, 10 and 20 degree, respectively.

As shown in Fig. 10, which simulates the layer number of 15 for reflectance with respect to visible light wavelength, the fluctuation at whole wavelength range observed, although the minimal reflectance is over 60%.

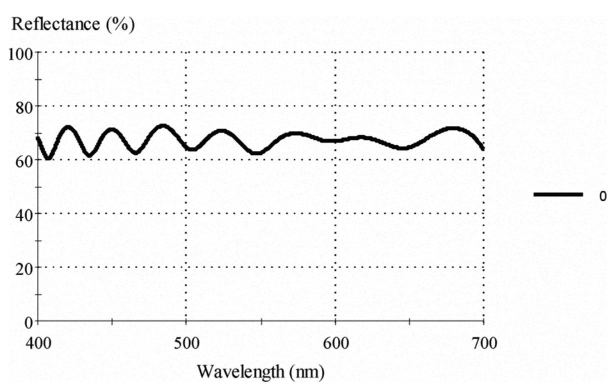

Fig. 10 Reflectance vs wavelength at layer number of 15 and incident angle of 0 degree.

From the comparison of effect of incident angle, it showed that 0 degree or vertical light incidence will have much better reflectance flatness, while the larger the angle, the larger of fluctuation in reflectance will be obtained; From the comparison for effect of layer number on reflectivity, it showed that the larger the number, the better the reflectivity in terms of flatness and value for each wavelength. However, the reflectivity in the whole visible light bandwidth (wavelength from 400 to 700nm) is around 60% with variation range of around 10%, which matches well with the measured results as reported in literature. It showed that the proposed model can be applied to explain the formation mechanism of bright whiteness in beetle scale.

On the other hand, it is obvious that the physical model can support only reflective mechanism of light propagation for interference, other phenomena such as light scattering and diffraction are not considered in this work. And the work here is for only one scale as the scales in the beetle have flat shape so it is possible to align the direction of multilayer scales which increases the effective reflectivity.

IV. Conclusions

A multi-layer film model is proposed for simulating the visible light reflection from beetle scale. Though the model and simulation analysis, it showed that the simulated results can explain the observed bright white phenomena very well with the variation of layer number and layer thickness by alteration of the air-layer and chitin layer. It is concluded that the model is reliable and can be applied for design of bright white biomimetic thin film coating materials. Further theoretical work will be continued for refining the model and optimizing the design for the high-brightness optical composite films or coating materials, and fabricating work for novel materials is also expected following the optimal design.

Acknowledgment

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