## Near-infrared photon propagation in complex knee by Monte-Carlo modeling

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It is highly necessary to study the phenomenon of photon migration in the knee joint for the non-invasive near-infrared optical early diagnosis of the osteoarthritis of the knee. We investigate the migration trace and distribution rule of the photons in knee layered structure, which are simulated by the Monte-Carlo modeling. The proportion of photons which collide with bone tissue then migrate out of the muscle tissue and photons directly migrate out of muscle tissue is calculated. For analyzing the signal-to-noise ratio to determine the accurate position of the detector, we perform quantitative evaluations of distribution of photons, as well as qualitative assessments of the distribution of photons.

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Osteoarthritis of the knee (KOA) is one of the most prevalent chronic diseases that severely affect the patients' quality of life and economy. There are some limitations in conventional clinical imaging techniques used in the diagnosis of osteoarthritis<sup>[1,2]</sup>. Near-infrared spectroscopy (NIRS) is an important method to measure the changes that occur in the composition of complex composites<sup>[3]</sup>. It is necessary to study the phenomenon of photon migration in the knee joint in the field of non-invasive near-infrared optical early diagnosis of the KOA<sup>[4]</sup>. It is very important to establish a propagation model which can accurately describe the migration of photons in the tissue. Monte-Carlo (MC) method has been regarded as a golden rule for studying the photon propagation in biological tissue<sup>[5,6]</sup>. Here, near-infrared beam is normally incident upon the surface of the knee joint, and the migration trace and distribution rule of photons are simulated by the MC method in knee layered structure, which mainly consists of muscle tissue and bone tissue with complex boundary. Photons, which finally migrate out of muscle, are analyzed. Those photons which collide with bone tissue are considered as a signal, and the others are noise. The proportion of signal to noise that can be applied to the KOA detection is analyzed.

Figure 1(a) shows the complex knee joint structure. As an initial research, knee joint can be divided into two parts according to its optical properties: bone tissue and muscle tissue, as shown in Fig. 1(b). Many studies have reported on the simulation process of MC method<sup>[7–9]</sup>. Based on these studies, a photon propagation model of the knee layered structure is proposed and the simulation flow chart is designed to deal with specific issues. The photon propagation model is shown in Fig. 1(b); and the flow chart for the MC simulation of photon propagation is shown in Fig. 2.

The length of a scattering step in each scattering point is uncertain. Photon's step of movement is determined by the mean free path of the cumulative probability distribution:

$$\Delta s = -\ln \xi / \mu_t, \tag{1}$$

where  $\xi$  is a random number from the uniform distribution of (0, 1).

The photon will be absorbed or scattered during the movement. Absorption decays the photon package weight, that is, the amount of the weight loss:

$$\Delta w(n,m) = w(n,m-1) * \mu_{\rm a}/\mu_{\rm t}.$$
(2)



Fig. 1. (a) CT image of the knee joint; (b) Photon propagation model. Solid line represents the migration trace of photons which collide then migrate out of the muscle tissue. Dotted line represents the migration trace of photons which directly migrate out of the muscle tissue. White areas indicate bone tissue; gray areas indicate muscle tissue; and black areas indicate the external.



Fig. 2. Flow chart for the MC simulation of photon propagation.

Scattering changes the direction of photon transmission. The new transmission direction of photon is determined by the cumulative probability distribution of scattering angle  $\theta$ . The Henyey Greenstein phase function determines the probability distribution of the cosine of the scattering angle  $\theta$ :

$$p(\cos\theta) = (1 - g^2) / [2(1 + g^2 - 2 * g * \cos\theta)^{3/2}], \quad (3)$$

and the scattering angle  $\theta$  satisfies:

$$\cos \theta = \begin{cases} 2\xi - 1 & g = 0\\ \left\{ 1 + g^2 - \left[ (1 - g^2) / 1 - g + 2g\xi \right]^2 \right\} / (2g) g \neq 0.$$
(4)

Optical properties of the knee joint present complexity due to differences in the individual, and parameters of optical properties among various components are different. In mammals, the refractive index lies in the range of 1.37–1.39 (except fat), and the refractive index of adipose tissue is  $1.45^{[10]}$ . Owing to the different refractive indices of various compositions, different events occur. Muscle is a typical tissue with strong scattering and weak absorption features. When the photon packet collides with muscle tissue boundary, total reflection or transmission occurs. If the reflectivity is greater than the number  $\xi$ , then total reflection occurs; if reflectivity is less than the number  $\xi$ , the photon packet migrates out of the boundary. The reflectivity is given by the Fresnel formula:

$$R(a_{i}) = [\sin^{2}(a_{i} - a_{t})/\sin^{2}(a_{i} + a_{t}) + \tan^{2}(a_{i} - a_{t}) / \tan^{2}(a_{i} + a_{t})]/2,$$
(5)

where  $a_i$  is the angle of incidence, which can be calculated by two straight angle formulas;  $a_t$  is the angle of refraction, which can be calculated by Snell's law. When the photon packet transmission occurs at the boundary, new coordinate is marked as (e, f). The number of transmitting photon and the gray level increase according to the weight change. As the bone tissue is a total reflection tissue, total reflection occurs at the boundary of bone tissue. The process of photon packet colliding with the boundary is shown in Fig. 3.

If the photons migrate out of the muscle boundary, it is considered as natural extinction. With light weight than a certain threshold value  $w_{\rm th}$  (in this letter  $w_{\rm th} = 0.00001$ ), the photon package will not be further studied in principle. In order to maintain a constant total energy of photon package, the "roulette wheel" method is used to determine whether to continue to track the photon packet<sup>[11,12]</sup>.

Tracing of migration of the emitted photons from the near-infrared light source within the knee has been simulated by the MC method, as shown in Fig. 4(a). Green dots indicate photons that collide with bone tissue then migrate out of the muscle tissue (CP). Red



Fig. 3. Process of photon packet colliding with the boundary.  $R_1$  and  $R_2$  represent the nearest boundary points. The intersection (e, f) can be calculated, which is the point at which the photon packet meets the interface while moving along the current direction. Then, the symmetry point (x', y'), which is out of the bound point  $(x_2, y_2)$  about the boundary line  $(R_1 - R_2)$ , is considered as the new coordinate point (photon symmetric boundary coordinate). The process mentioned above is repeated when the photon packet arrives at the boundary again.



Fig. 4. (a) Migration trace of photons; (b) intensity distribution of photons; (c) distribution fitting curve of photons; and (d) intensity distribution of photons of part and right parts.

dots indicate the photons that directly migrate out of the muscle tissue (DP). Most of the photons migrate out of the knee joint from the incident direction. These photons are of two types: CP and DP. The focus here is to detect CP. Photons that collide with bone tissue are considered as a signal, and the others are noise. The intensity distribution of 1000000 photons from light source is expressed by RGB color, as shown in Fig. 4(b). The deeper the red, heavier the weight of photons that collide with bone tissue then migrate out of the muscle tissue; the deeper the green, heavier the weight of photons that migrate out of the muscle tissue. Results show that only a small amount of the photons are detected after being absorbed and scattered by the knee joint. The detected photons of significance are less, which mainly concentrate in two portions S1 and S2, as shown in Fig. 4(b). The meaningful reflectance photons are relatively small. There are only two ways to make up: increasing light source photon injection and locating the detector at the optimal position at which more photons can be received. The fitting curve of distribution of photons is shown in Fig. 4(c). Intensity distribution of photons of left and right parts is shown in Fig. 4(d). The longer the distance from the center position, the fewer photons.

With the above analysis, we can roughly obtain positions S1 and S2. For analyzing the signal-to-noise ratio (SNR) to determine the accurate position of the detector, we performed quantitative evaluations of distribution of photons, as well as qualitative assessments of the distribution of photons. The proportion of CP to DP from left side of knee is shown in Fig. 5.

$$SNR = \frac{CP}{CP + DP} * 100\%.$$
(6)



Fig. 5. (a) Number distribution curve of photons which migrate out of the muscle tissue weight; (b) number distribution curve of photons which collide with bone tissue then migrate out of the muscle tissue; (c) proportion of photons which collide with bone tissue then migrate out of the muscle tissue and photons migrate out of muscle tissue. The proportion is the highest within the range of 50–100 pixels of the X-axis.

From Fig. 5(c), it can be seen that the part with an ideal SNR is in the range of 50–100 pixels in the X-axis, where the proportion is higher than the other place. These results are consistent with the qualitative analysis results. It is a theoretical basis for the detector to be placed, which will be more conducive to early detection of KOA.

Although the mechanism of interaction of light with the knee joint is very complex, the results simulated by the MC method are ideal. Either from the qualitative or quantitative perspective of analysis, the detector should be placed in that position: their conclusions are consistent. We consider more components of knee to simulate photon migration by the MC method in the future. And then, various structural shapes of optical inspection systems can be designed to place in the suitable position.

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