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Supplementary Material to "Poly(lactic acid) Films Reinforced with TiO_2 and ZnO Nanoparticles: Thermal, Mechanical, Optical, and Phytotoxicity Assessment"

Calculation of Color Difference by CIEDE2000 formula

The color difference (ΔE^*_{00}) between the backgrounds and the system composed of the polymeric film over the backgrounds was calculated using the CIEDE2000 equation (Equation S1), following the algorithm proposed by Sharma et al.[1], reproduced in this supplementary material. The CIEDE2000 equation employs the colorimetric parameters L^*, a^*, and b^* from the CIELab color space to compute perceptible color differences, converting them into the derived quantities lightness (L'), chroma (C'), and hue angle (h'), which are used in the terms of Equation S1.

$$\Delta E^*_{00} = \sqrt{\left(\frac{\Delta L'}{k_L \times S_L}\right)^2 \times \left(\frac{\Delta C'}{k_C \times S_C}\right)^2 \times \left(\frac{\Delta H'}{k_H \times S_H}\right)^2 + R_T \times \left(\frac{\Delta C'}{k_C \times S_C}\right) \times \left(\frac{\Delta H'}{k_H \times S_H}\right)} \qquad \text{(S1)}$$

For two distinct color points defined by the parameters L^*_i, a^*_i, and b^*_i ($i = 1, 2$) in the CIELab color space, the values of C'_i and h'_i were obtained through the sequence of calculations represented by Equations S2 to S7.

$$C^*_i = \sqrt{\left(a^*_i\right)^2 + \left(b^*_i\right)^2}\ ,\ i = 1, 2 \qquad \text{(S2)}$$

$$\overline{C^*} = \frac{C^*_1 + C^*_2}{2} \qquad \text{(S3)}$$

$$G = 0.5 \times \left(1 - \sqrt{\frac{\overline{C^{*'}}^{7}}{\overline{C^{*}}^{7} + 25^{7}}}\right) \tag{S4}$$

$$a_i^{'} = (1 + G) \times a_i^{*} \ , i = 1,2 \tag{S5}$$

$$C_i^{'} = \sqrt{(a_i^{'})^2 + (b_i^{*})^2} \ , i = 1,2 \tag{S6}$$

$$\begin{matrix} h_i^{'} = 0 \ , if \ b_i^{*} = a_i^{'} = 0 \\ h_i^{'} = \tan^{-1}(b_i^{*}, a_i^{'}), otherwise \end{matrix} , i = 1,2 \tag{S7}$$

From the L_i^*, $C_i^{'}$, and $h_i^{'}$ data, the differences in lightness ($\Delta L^{'}$), chroma ($\Delta C^{'}$), and hue ($\Delta H^{'}$) were calculated using Equations S8 to S11.

$$\Delta L^{'} = L_2^{*} - L_1^{*} \tag{S8}$$

$$\Delta C^{'} = C_2^{'} - C_1^{'} \tag{S9}$$

$$\begin{aligned} &\Delta h^{'} = 0 \ , if \ C_1^{'} \times C_2^{'} = 0 \\ &\Delta h^{'} = h_2^{'} - h_1^{'} \ , if \ C_1^{'} \times C_2^{'} \neq 0 \ and \ \left|h_2^{'} - h_1^{'}\right| \leq 180° \\ &\Delta h^{'} = \left(h_2^{'} - h_1^{'}\right) - 360° \ , if \ C_1^{'} \times C_2^{'} \neq 0 \ and \ \left(h_2^{'} - h_1^{'}\right) > 180° \\ &\Delta h^{'} = \left(h_2^{'} - h_1^{'}\right) + 360° \ , if \ C_1^{'} \times C_2^{'} \neq 0 \ and \ \left(h_2^{'} - h_1^{'}\right) < -180° \end{aligned} \tag{S10}$$

$$\Delta H^{'} = 2 \times \sqrt{C_1^{'} \times C_2^{'}} \sin\left(\frac{\Delta h^{'}}{2}\right) \tag{S11}$$

The weighting factors S_L, S_C, and S_H, as well as the rotation term R_T, were obtained through the sequence of calculations described by Equations S12 to S21.

$$\overline{L'} = \frac{\left(L_1^* + L_2^*\right)}{2} \tag{S12}$$

$$\overline{C'} = \frac{\left(C_1' + C_2'\right)}{2} \tag{S13}$$

$$\begin{aligned}
&\overline{h'} = \left(h_1' + h_2'\right), \mathit{if}\ C_1' \times C_2' = 0 \\
&\overline{h'} = \frac{h_1' + h_2'}{2}, \mathit{if}\ C_1' \times C_2' \neq 0\ \mathit{and}\ \left|h_1' - h_2'\right| \leq 180° \\
&\overline{h'} = \frac{\left(h_1' + h_2'\right) + 360°}{2}, \mathit{if}\ C_1' \times C_2' \neq 0\ \mathit{and}\ \left|h_1' - h_2'\right| > 180° \mathit{and}\ \left(h_1' + h_2'\right) < 360° \\
&\overline{h'} = \frac{\left(h_1' + h_2'\right) - 360°}{2}, \mathit{if}\ C_1' \times C_2' \neq 0\ \mathit{and}\ \left|h_1' - h_2'\right| > 180° \mathit{and}\ \left(h_1' + h_2'\right) \geq 360°
\end{aligned} \tag{S14}$$

$$\begin{aligned}
T &= 1 - 0.17 \times \cos\left(\overline{h'} - 30°\right) + 0.24 \times \cos\left(2 \times \overline{h'}\right) + \\
&+ 0.32 \times \cos\left(3 \times \overline{h'} + 6°\right) - 0.20 \times \cos\left(4 \times \overline{h'} - 63°\right)
\end{aligned} \tag{S15}$$

$$\Delta\theta = 30° \times \exp\left[-\left(\frac{\overline{h'} - 275°}{25°}\right)^2\right] \tag{S16}$$

$$R_C = 2 \times \sqrt{\frac{\overline{C'}^7}{\overline{C'}^7 + 25^7}} \tag{S17}$$

$$S_L = 1 + \frac{0.015 \times \left(\overline{L'} - 50\right)^2}{\sqrt{20 + \left(\overline{L'} - 50\right)^2}} \tag{S18}$$

$$S_C = 1 + 0.045 \times \overline{C'} \quad \text{(S19)}$$

$$S_H = 1 + 0.015 \times \overline{C'} \times T \quad \text{(S20)}$$

$$R_T = -\sin(2 \times \Delta\theta) \times R_C \quad \text{(S21)}$$

Finally, the parameters k_L, k_C, and k_H were assigned the values 2, 1, and 1, respectively, as recommended by Cinko and Becerir[2].

References

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