Flake Color Simulation

Karl Falb - falb.karl@columbia.edu

Introduction

This site roughly simulates the color of an exfoliated 2D material on a silicon substrate (when viewed under a microscope). The three dials allow you to adjust illuminating light color temperature, flake thickness, and illuminating light intensity. Flake material and SiO_2 thickness can be chosen from the drop-down menus.
The colors are calculated roughly as follows. The reflectance of the thin-film system (air + flake + SiO_2 + silicon substrate) is multiplied by the spectral radiance of the incident light (assumed to be a black-body) to get the observed spectrum of light. Then, to map the spectrum to a three-value color space (say sRGB), for each value, the spectrum is weighted by some weighting function, integrated over, and normalized with a common normalization factor.
The process of mapping the spectrum to an sRGB value can vary. This site uses a human perceptual model (following CIE 1931 XYZ, then converting to sRGB), but to simulate a microscope camera, the camera sensor data sheet should specify RGB channel sensitivity across different wavelengths. This is to say, this is indending to simulate what you would see as you look at a flake through a microscope, not what a picture of the flake would look like. Feel free to fact-check me on any of this.

Reflectance

Following the method in §2.3-§2.4 of MacLeod's *Thin Film Optical Filters* (the first source I found), the reflectance is calculated as follows.

$$\begin{bmatrix} B \\ C \end{bmatrix} = \left\{ \prod_{r=1}^{q} \begin{bmatrix} \cos\delta_r & (i\sin\delta_r)/\eta_r \\ i\eta_r \sin\delta_r & \cos\delta_r \end{bmatrix} \right\} \begin{bmatrix} 1 \\ \eta_m \end{bmatrix} \tag{1}$$

$$R = \left| \frac{\eta_0 - C/B}{\eta_0 + C/B} \right|^2 \tag{2}$$

where the indices correspond to the layers in the system: air (0), thin films (1) ... (q), substrate (m), and variables are defined as follows

$$\delta_i = 2\pi N_i d_i/\lambda \tag{3}$$

$$\eta_i = N_i\sqrt{\epsilon_0/\mu_0} \tag{4}$$

where $\{d_i\}$ are thicknesses of the films and $N_i(\lambda) = n_i(\lambda) - ik_i(\lambda)$ are the complex refractive indices of your materials. Thus reflectance is a function of the system geometry, incident light wavelength λ, and the complex refractive indices of the materials, which are in turn a function of λ.

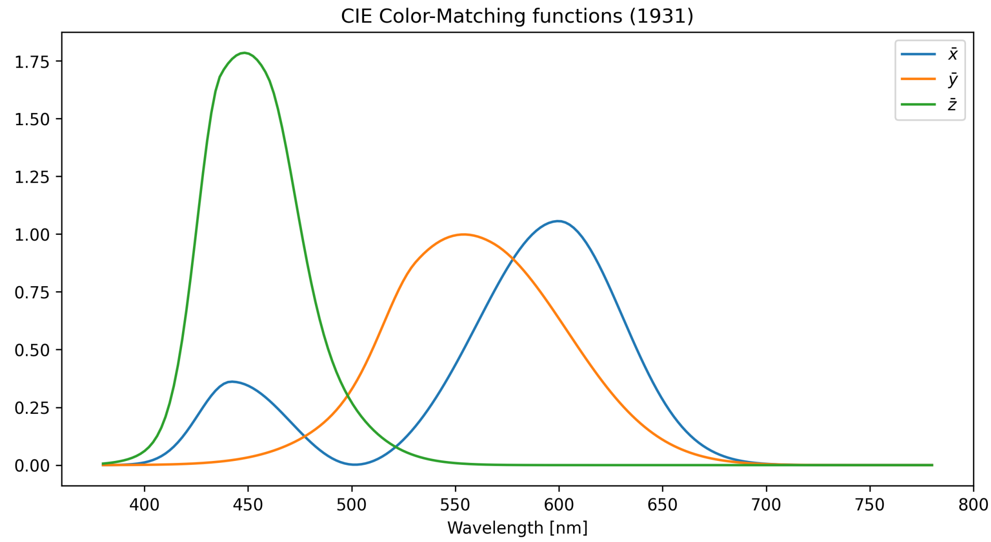

Figure 1: Weighting functions for XYZ color space

sRGB

One can look up the CIE 1931 XYZ for more information, but essentially the process here maps the spectrum to XYZ color space, which can be mapped to sRGB with a matrix transformation, application of a gamma function, and cuts to ensure [0, 1] limits.

$$X = \frac{L}{N} \int_\Lambda I(\lambda) R(\lambda) \bar{x}(\lambda) \, \mathrm{d}\lambda \tag{5}$$

$$Y = \frac{L}{N} \int_\Lambda I(\lambda) R(\lambda) \bar{y}(\lambda) \, \mathrm{d}\lambda \tag{6}$$

$$Z = \frac{L}{N} \int_\Lambda I(\lambda) R(\lambda) \bar{z}(\lambda) \, \mathrm{d}\lambda \tag{7}$$

$$N = \int_\Lambda I(\lambda) \bar{y}(\lambda) \, \mathrm{d}\lambda \tag{8}$$

where $I(\lambda)$ is the spectral radiance of the incident light (taken in this simulation to be a black-body with temperature T, $I(\lambda, T)$), $\bar{x}$ $\bar{y}$ $\bar{z}$ are the weighting functions, $\Lambda \in [380, 780]$nm, and L is some measure of relative light intensity. $\bar{y}$ corresponds to the luminance, the human perception of which is brightness, so it is used with the incident spectral radiance to normalize the XYZ values.

$$\begin{bmatrix} R \\ G \\ B \end{bmatrix}_{\mathrm{sRGB}} = \mathrm{constrain}_{[0,1]} \left(\gamma \left(\begin{bmatrix} 3.2404542 & -1.5371385 & -0.4985314 \\ -0.9692660 & 1.8760108 & 0.0415560 \\ 0.0556434 & -0.2040259 & 1.0572252 \end{bmatrix} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} \right) \right) \tag{9}$$

$$\gamma(x) = \begin{cases} 12.92x & \text{if } x \leq 0.0031308 \\ 1.055x^{1/2.4} - 0.055 & \text{otherwise} \end{cases} \tag{10}$$

$$\text{constrain}_{[0,1]}(x) = \begin{cases} 1 & \text{if } x > 1 \\ 0 & \text{if } x < 0 \\ x & \text{otherwise} \end{cases} \tag{11}$$