

Film the Film

A new method to measure oxygen diffusion in polymer films using light.

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Problem

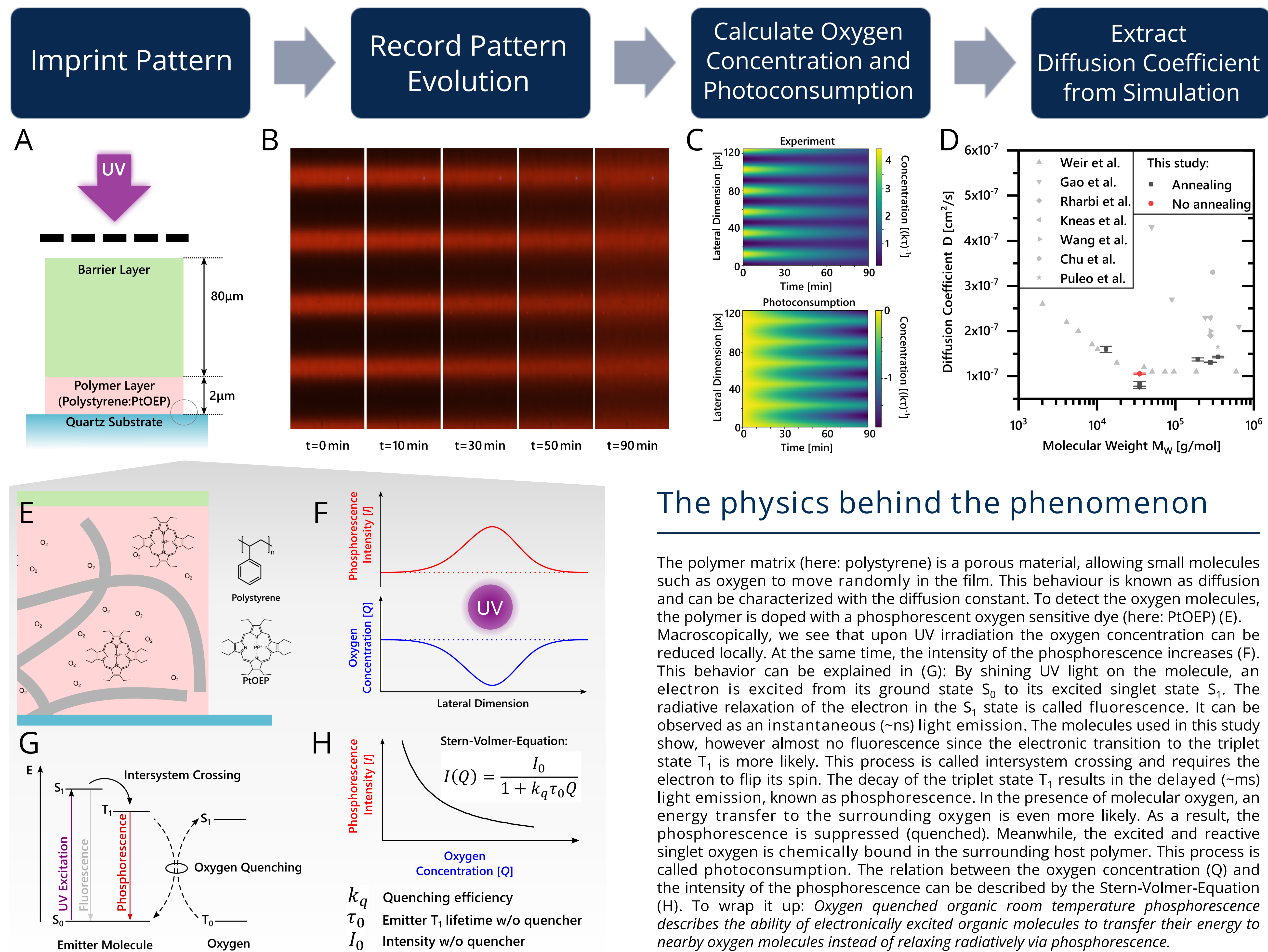
Organic materials such as polymer films surround us in many everyday applications ranging from food packaging and smartphone OLED displays to medical purposes. One of their main usage scenarios is the thin, lightweight, and easy processable encapsulation to protect a particular target from molecular oxygen. Hence, the oxygen diffusion properties in these polymer films represent a key parameter.

Goal

This work aims to demonstrate a new method to determine the oxygen diffusion coefficient in thin polymer films using light. The concept should be tested at the exemplary case of polystyrene.

Conception

The polymer layer is covered with an oxygen impermeable barrier layer (Exceval™) and doped with organic dye molecules (PtOEP). This system is known as programmable luminescent tag (PLT). It allows to imprint a luminescent pattern in the polymer layer using 365 nm UV light and a shadow mask (A). The exploited effect is called oxygen quenched room temperature phosphorescence. By recording how the pattern blurs over time with a CCD-camera, we can track how oxygen molecules from the dark areas penetrate the bright areas (B). From the pixel values of the image series, the oxygen concentration and the amount of photoconsumed oxygen is calculated (C). The experimental data is fitted with a diffusion simulation yielding the oxygen diffusion constant and compared to literature (D).



The physics behind the phenomenon

The polymer matrix (here: polystyrene) is a porous material, allowing small molecules such as oxygen to move randomly in the film. This behaviour is known as diffusion and can be characterized with the diffusion constant. To detect the oxygen molecules, the polymer is doped with a phosphorescent oxygen sensitive dye (here: PtOEP) (E). Macroscopically, we see that upon UV irradiation the oxygen concentration can be reduced locally. At the same time, the intensity of the phosphorescence increases (F). This behavior can be explained in (G): By shining UV light on the molecule, an electron is excited from its ground state S_0 to its excited singlet state S_1 . The radiative relaxation of the electron in the S_1 state is called fluorescence. It can be observed as an instantaneous (\sim ns) light emission. The molecules used in this study show, however almost no fluorescence since the electronic transition to the triplet state T_1 is more likely. This process is called intersystem crossing and requires the electron to flip its spin. The decay of the triplet state T_1 results in the delayed (\sim ms) light emission, known as phosphorescence. In the presence of oxygen, an energy transfer to the surrounding oxygen is even more likely. As a result, the phosphorescence is suppressed (quenched). Meanwhile, the excited and reactive singlet oxygen is chemically bound in the surrounding host polymer. This process is called photoconsumption. The relation between the oxygen concentration (Q) and the intensity of the phosphorescence can be described by the Stern-Volmer-Equation (H). To wrap it up: *Oxygen quenched organic room temperature phosphorescence describes the ability of electronically excited organic molecules to transfer their energy to nearby oxygen molecules instead of relaxing radiatively via phosphorescence.*

Results

The method was tested for the model system polystyrene with 6 different molecular weights ranging from $1,3 \times 10^4$ g/mol to $3,5 \times 10^5$ g/mol (D). The values lie well in the range reported in the literature. For polystyrene with $M_w = 3,5 \times 10^4$ g/mol, two different processing conditions (i.e. with annealing and w/o annealing) were investigated. Our study indicates a strong dependency of the diffusion coefficient on the processing conditions. We found $D = (1,49 \pm 0,08) \times 10^{-7}$ cm²/s for unannealed and $D = (0,71 \pm 0,09) \times 10^{-7}$ cm²/s for annealed samples. Common methods to determine the oxygen diffusion coefficient usually rely on heavy and expensive vacuum technology. In contrast, our procedure provides a significant advantage: No vacuum machinery is needed.

More

Scanning the QR code, you can find:

- ✓ List of references
- ✓ Key literature on programmable luminescent tags (PLTs)
- ✓ Digital Version of this poster
- ✓ Supplementary Material
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