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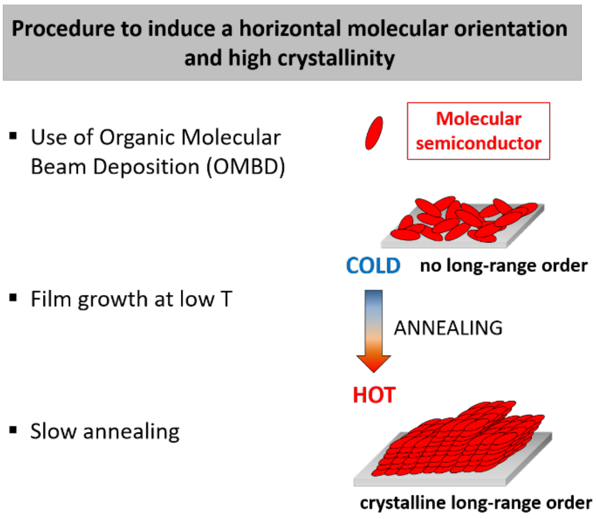
A new method to induce a stable horizontal molecular orientation in crystalline thin films of organic semiconductors

Technology Description



Procedure to induce a horizontal molecular orientation and high crystallinity

- Use of Organic Molecular Beam Deposition (OMBD)
- Film growth at low T
- Slow annealing

The invention concerns a new preparation method for polycrystalline thin films of rod-like molecular organic semiconductors. Resulting films are highly crystalline with a horizontal orientation of the semiconducting molecules, i.e. long molecular axis parallel to the substrate plane.
The new route includes vacuum-deposition of the organic material on a substrate, which is cooled down to a suitable temperature to suppress molecular dynamics. At this stage the molecules align in an overall horizontal orientation while the film still lacks long-range order. Thermal annealing close to the material desorption temperature induces strong crystallization of the film, with the molecules staying "kinetically trapped" in their horizontal orientation under environmental conditions.

Innovation

Up to now: "Glassy" films or liquid crystal-like films, possible to obtain an average horizontal molecular orientation but exhibiting a broad distribution. Lack of long-range order in the directions parallel (in-plane) and perpendicular (out-of-plane) to the substrate plane at the same time.

Now: Polycrystalline, uniaxially anisotropic films with high coherence length in both in-plane and out-of-plane directions. Well-defined horizontal molecular orientation with narrower distribution. Flexibility in the choice of material/substrate.

Market Potential / IP Status

We see a huge market potential as the method is applicable to a wide field of applications with a variety of substrates (both amorphous and crystalline) and molecular materials (see Duva et al.). The method fits vacuum processing requirements for production and the processed films are stable under environmental conditions.

Patent filed – Submission date 2018-08-15.

Applications

☐ **Organic and Hybrid Solar Cells**
☐ **Light Sensors**
☐ **Organic Field-Effect Transistors**
☐ **Gas Sensors**

Advantages

☐ Fabrication method compatible with vacuum processes
☐ Control of film morphology depending on annealing temperature
☐ Higher light absorption efficiency
☐ High flexibility in the choice of the molecular material + substrate combination

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METHOD

Sample Preparation – Diindenoperylene (DIP)

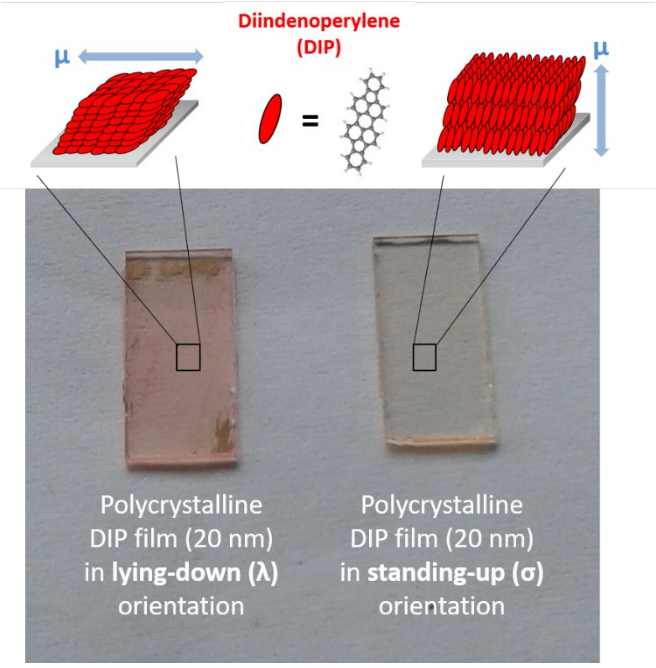

Fig. 1: Diindenoperylene thin films deposited by means of Organic Molecular Beam Deposition on glass slides.

The film thickness controlled by a calibrated quartz-crystal microbalance is 20 nm and has been cross-checked with AFM and X-ray reflectivity.

The sample on the left has been prepared using the procedure developed to induce a lying-down (horizontal) molecular orientation of polycrystalline films (see Duva et al., 2019).

The sample on the right has been prepared under conditions similar to Heinemeyer et al., 2008.

Quantitative UV-vis absorption data on these films show that the absorptivity of lying-down Diindenoperylene (DIP) is roughly four times higher than for standing-up DIP (see Fig. 2). The increased light absorption efficiency of lying-down DIP is clear already at a first visual inspection of the two representative samples put on a white paper and illuminated with environmental light.

Demonstration Measurement – DIP

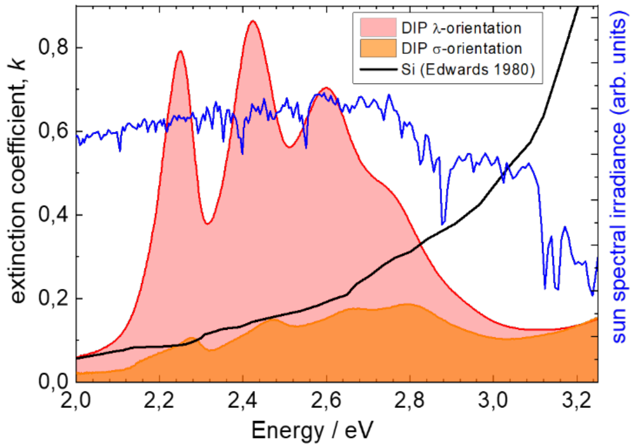

Fig. 2: UV-vis transmission measurements in the visible range for the same DIP films shown in Fig.1. The extinction coefficient of Silicon is reported for comparison, together with the sun spectral irradiance on Earth. Adapted from Duva et al., 2019.

The in-plane component (i.e. parallel to the substrate plane) of the extinction coefficient, $k_{||}$, in the visible range is 4-5 times higher for lying-down (λ) DIP compared to standing-up (σ) DIP. This can be explained considering that the λ-orientation of the molecules on the substrate allows maximising the coupling of the HOMO-LUMO transition dipole moment (μ) with the radiation in normal incidence. This allows to compensate for the low extinction of Silicon in the visible range, where the sun irradiance is highest (Fig. 2), in ultra-thin Si solar cells, further increasing their efficiency. Note that also in the UV range (≈ 3.5 – 6 eV) $k_{||}$ is higher for lying-down DIP approx. by a factor of two (see Duva et al., 2019).

REFERENCES

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