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## **HOLE DRIFT MOBILITY IN ANTRACHINON LAYERS**

*The drift mobility of holes in the antrachinon layers were determined. The layers were evaporated in the vacuum of the order of  $10^{-5}$  Torr. Due to the substrate temperature the layers were in the structure polycrystalline or the quasi-amorphous. There were no obtained the effect of the layers structure on the magnitude of the mobility of the carriers and on the transport mechanism.*

**Keywords:** polycrystalline and quasi-amorphous antrochinone films, hole drift mobility, carrier transport.

### **1. INTRODUCTION**

Organic molecular crystals in the type of thin films and aggregates are technologically in the electronic meaning very attractive materials.

Their usefulness relies to a large extent on their photoconductivity, light absorption, non-linear polarizability etc., i.e. the properties immediately related to the electronic structure of these materials. A rigorous quantum mechanical treatment of a crystal requires determination of its band structure within periodic boundary conditions. Such the calculations for the crystals built up of the large sized molecules is very difficult and sometimes is not possible without the coarsened approximations.

One of the possible path for by-pass this problem is a limitation the quantum mechanical treatment to an individual molecule and then to consider the intermolecular interactions in terms of the self consistent reaction field. The molecular properties can be used as the input parameters in calculations of solid

state properties, such a energetic structure of the forbidden gap and can be verify by an experiment [1, 2].

Molecular electrostatic potential (MEP) is formed by contribution from atomic charges, dipoles the higher multipole moments vanish by symmetry [3]. If a molecular crystal is formed only by the van der Waals interactions, the shortest intermolecular separations C...H and C...C are 2,8 – 2,9 Å and 3,3 – 3,4 Å, respectively. At the distances of this range, the contributions from atomic quadruple moments can be neglected and for calculations of the crystalline electrostatic potential only atomic point charges and point dipoles may be used.

In some molecular crystals the effect of the crystal structure exceeds the effect of hydrogen bonding and is directed oppositely to it; thus the total effect of crystalline electrostatic potential reduce the molecular dipole moment [4]. There were taken tests for check how the dipole moment of the molecules of the molecular crystal or their absence effect on the mechanism of the charge carriers transport. For this reason there were chosen two molecular crystals with nearly identical crystalline structure. The first was the antron, which molecules are with the dipole moment. The second was the antrachinon, which molecules are with the nearly zero dipole moment. As the first there were made the experiments on the carrier mobility for the antrachinon layers.

## 2. EXPERIMENTAL

The structure of antrachinon,  $C_{14}H_8O_2$ , has been repeatedly investigated, most recently at several temperatures between  $-170^{\circ}C$  and  $20^{\circ}C$ . Its crystals are monoclinic with bimolecular unit of the dimensions (in room temperature):  $a_0 = 15,810(15)$  Å,  $b_0 = 3,942(5)$  Å,  $c_0 = 7,865(10)$  Å,  $\beta = 102^{\circ}43(2)'$ . The space group  $C_{2h}^5(P2_1/a)$  places its atoms in the positions:  $(4e) \pm(xyz; x+1/2, 1/2 - y, z)$ .

Planar, centrosymmetric molecules have the bond dimensions shown in the Fig. 1 with the distances C-H lying between 1,00 and 1,04 Å. The antrachinon molecule posses a natural dipole moment measured in benzene 0,6 D ( $2,00 \cdot 10^{-30}$  Cm) [5], and computed from the Chyperchem programme the worth is 0,00079 D (that is that it practically equals zero). The films were evaporated with spectral grade antrachinon (obtained with zone melting).

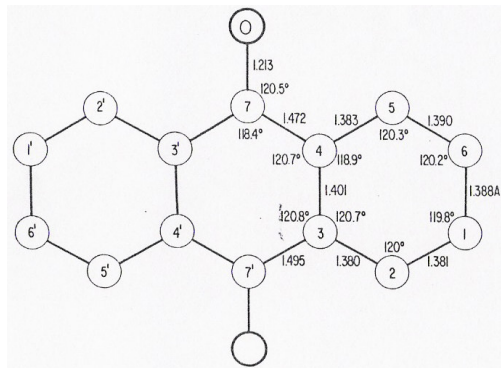


Fig. 1. Bond dimensions in the molecule of anthracinon [5]

The anthracinon samples were obtained by evaporation in vacuum under the pressure of the order of  $10^{-5}$  Torr on glass plates. The substrate temperature was for polycrystalline layers was about 300 K, and for quasi-amorphous layers the substrate temperature was 170 – 200 K and with proper evaporation rate. Structural examination obtained anthracinon layers was made using X – ray diffraction. In order to attain that one employed an automatic diffractometer DAR. Diffraction examinations were made in the  $2\theta$  range from  $5^\circ$  to  $80^\circ$  with measuring step  $0,05^\circ$ . Typical diffraction patterns for the tested polycrystalline and quasi-amorphous films are described with Fig. 2.

For polycrystalline and quasi-amorphous layers there were made the examinations of the drift mobility of holes using the time of flight set-up working under computer control which enables to control the measurements and to store the data. The time of flight was found from the current signal. the current pulses were measured with digital oscilloscope DSO 5804. The system is completely described in [6-9].

Typical current pulse obtained for the polycrystalline anthracinon layers is presented in Fig. 3.

The examinations on the hole mobility for the polycrystalline anthracinon layers were made in the limits of the electrical field from  $1 \cdot 10^{-3}$  V/cm to  $5 \cdot 10^4$  V/cm. The investigations were made in the room temperature and the results are presented in Fig. 4. The determination of the activation energy of the mobility for these layers was made in the temperature limits 270 – 360 K. The results of these investigations are shown in the Fig. 4 too.

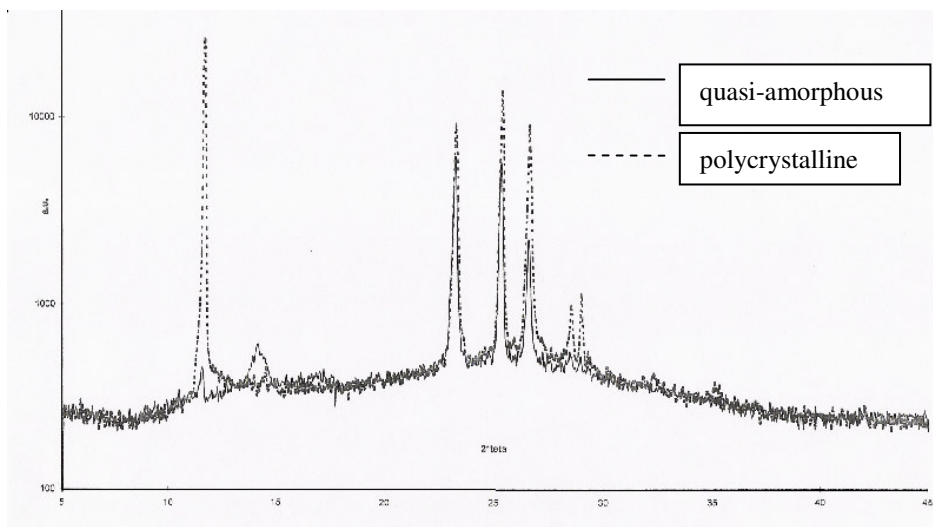


Fig. 2. Diffraction pattern (X-ray) for tested polycrystalline and quasi-amorphous anthracinon layers

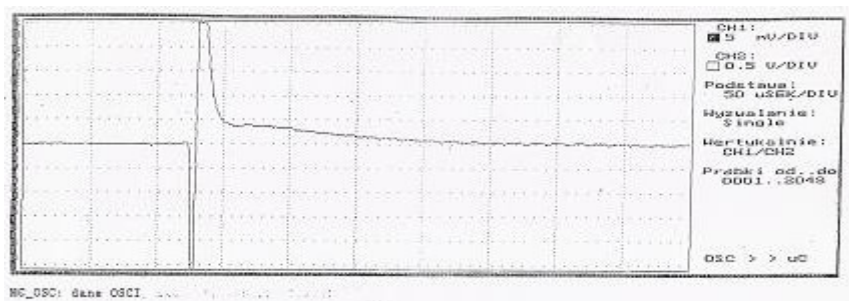


Fig. 3. Typical current pulse for polycrystalline anthracinon layers

For the polycrystalline anthracinon layers there were obtained the mobilities for holes in the range  $(8 \pm 2) \cdot 10^{-4} \text{ cm}^2/\text{Vs}$  and the activation energy for mobility on the level of  $kT$ , that is 0,03 eV. For quasi-amorphous anthracinon layers there were obtained with the TOF experiment the current pulses very similar with the current pulses obtained for polycrystalline layers (see Fig. 3). The example of the value for the mobility of the quasi-amorphous layer is shown in the Fig. 5. Generally it can be say that the values of the mobility for the quasi-amorphous anthracinon layers were with a great spread, and were limited in the range  $(3 - 7) \cdot 10^{-4} \text{ cm}^2/\text{Vs}$ .

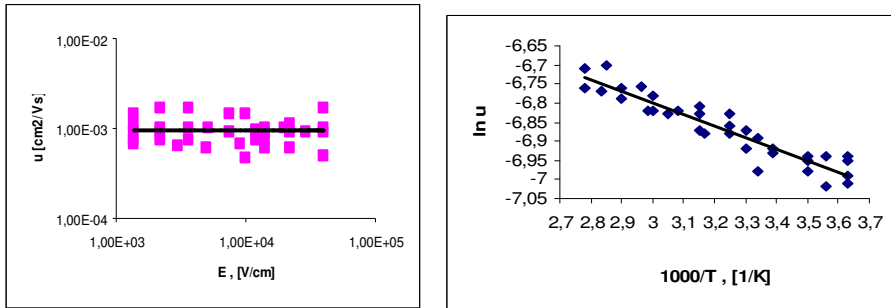


Fig. 4a). Hole drift mobility in polycrystalline anthracinon layer; b) Temperature dependence of the mobility for anthracinon layer

The value of the activity energy for mobility were determined only in the small range of temperatures, and it can be supposed in the range of  $kT$ . For the polycrystalline materials when the transport is controlled by the traps, the drift mobility can be described with the formula:  $\mu_d(T) = a T^{-n} \cdot b \exp(-E_t/kT)$ , where  $E_t$  is the mean depth of the traps. If in this formula the second term dominates, then the mobility dependence has the identical shape as for the hopping transport:  $\mu_d(T) \approx \exp(-E_h/kT)$ , where  $E_h$  is the activation energy for hopping [9, 10].

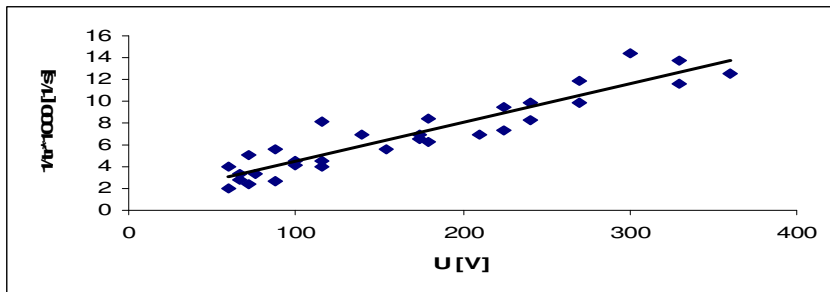


Fig. 5. Inverse time of flight due to the voltage applied to the quasi-amorphous anthracinon layer

### 3. CONCLUSIONS

For anthracinon layer, which molecules are without the dipole moment, there were determined that:

1. the value of the hole mobility is in the order of  $10^{-4} \text{ cm}^2/\text{Vs}$  and a small worth of the activation energy for mobility on the level of  $kT$ ,

2. the hopping transport or the band transport is with participation of the traps,
3. there is the absence of the effect of the structure of the layer on the hole transport.

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## RUCHLIWOŚĆ DZIUR W WARSTWACH ANTRACHINONU

### Streszczenie

Badano ruchliwość dziur w polikrystalicznych i quasi-amorficznych warstwach antrachinonu. Określono typową dla acenów o takim stanie nieuporządkowania wartość ruchliwości. Na podstawie uzyskanych rezultatów nie można jednoznacznie określić z jakim mechanizmem transportu mamy do czynienia. Nie stwierdzono na tym poziomie nieuporządkowania wpływu struktury na mechanizm transportu, choć można się było tego spodziewać.