

**SYLWESTER KANIA<sup>1,2</sup>**

<sup>1</sup> Institute of Physics, Technical University of Łódź, Wólczańska 219  
90-924, Łódź, Poland

<sup>2</sup> Centre of Mathematics and Physics Technical University of Lodz  
Al. Politechniki 11, 90-924 Łódź, Poland

## **ELECTRON DRIFT MOBILITY IN ANTHRONE LAYERS**

*There were investigated the magnitude of the mobility and the type of the mechanism of the electron transport in the anthrone layers with a different grade of the structural order, namely in polycrystalline and quasi-amorphous layers. The anthron samples were obtained by evaporation in vacuum under the pressure of the order of  $10^{-5}$  Torr on glass plates with different substrate temperatures and with different evaporation rates. Structural examination of the obtained anthrone layers was made using X-ray diffraction. Drift electron mobility for obtained polycrystalline and quasi amorphous layers were determined with TOF method. Obtained results show the almost lack of the mobility dependence due to the magnitude of the disorder, although the other results should be expected. Both obtained mobility values, were less than  $10^{-2}$  cm<sup>2</sup>/Vs and activation energy value on the  $kT$  level but simultaneously estimated density of hopping states was relatively big. In this case it does not permit us to indicate the dominant transport mechanism.*

**Keywords:** quasi-amorphous, polycrystalline anthrone films, electron drift mobility, carrier transport.

### **1. INTRODUCTION**

Fundamental understanding of organic molecular condensed matter can open new perspectives in modern electronics. Opportunity of deep modulation of electronic parameters with low melting point is very interesting for material engineering. This requires an experimental knowledge about charge injection

and transport. Low melting temperature due to the van der Waals bonds is a thermodynamic source of huge amount of structural defects in the samples of such the materials. That is the reason for a different grade of structural order layers used in commercial electronics. This paper is devoted to the drift mobility in anthrone layers with different structural order, namely polycrystalline and quasi-amorphous. Anthrone possess permanent molecular dipole moment. And the fact that dipolar attraction can be in the same order of magnitude as the van der Waals component of bonding makes this material very interesting for the modulation of conductivity and is connected with the electronic structure of that material. A rigorous quantum mechanical treatment of an organic condensed matter requires determination of its band structure within periodic boundary conditions. Such the calculation 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 solution of 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 is formed by contribution from atomic charges, dipoles, and the higher multipole moments vanish by symmetry [3]. If a molecular crystal is formed only by the van der Waals interactions, then 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.

For some molecular organic 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 affect on the mechanism of the charge carriers transport. For this reason there were done studies on the two molecular crystals with nearly identical crystalline structure. The first was the anthron, which molecules possess the dipole moment. The second was the antrachinone, with the nearly zero dipole moment. As the first there were made the experiments on carrier mobility for the antrachinone layers and in the second the anthrone layers were examined.

## 2. EXPERIMENTAL AND RESULTS

The structure of anthrone,  $C_{14}H_{10}O_2$ , 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):  $a = (15.80 \pm 0.03) \text{ \AA}$ ,  $b = (3.998 \pm 0.005) \text{ \AA}$ ,  $c = (7.86 \pm 0.16) \text{ \AA}$  and  $\beta = 101^{\circ} 40'$  [5, 6].

The space group  $C_2H_5$  ( $P2_1/a$ ) places its atoms in the positions:  $\pm(xyz)$ ;  $\pm(x+1/2, 1/2 - y, z)$  with oxygens distributed statistically over half of these positions. Planar, with asymmetrical molecules have the bond dimensions shown in the Fig 1. The anthrone molecule possess a natural dipole moment measured in benzene 3,66 D ( $1,22 \cdot 10^{-29}$  Cm) [6].

The anthrone samples were obtained by evaporation in vacuum under the pressure of the order of  $10^{-5}$  Torr on glass plates. The substrate temperature was about 300 K for polycrystalline layers, and for quasi-amorphous layers the substrate temperature was 170-200 K with a proper evaporation rate. Structural examinations of obtained anthrone layers were made using X-ray diffraction. For this purpose the automatic diffractometer DAR was employed. 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 tested polycrystalline and quasi amorphous films are both described with Fig 2. For polycrystalline and quasi-amorphous layers there were made the examinations of the drift mobility of electrons 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 and Rigol DS1000CA. The system is completely described in [7-10, 15, 16].

TOF measurement of the electron mobility for the anthrone layers was considerable difficult because of the lack of electrical stability of the samples under study. Much more convenient were the measurements for hole mobility in those samples. Typical current pulse obtained for the electrons of the polycrystalline anthrone layers is presented in Fig. 3.

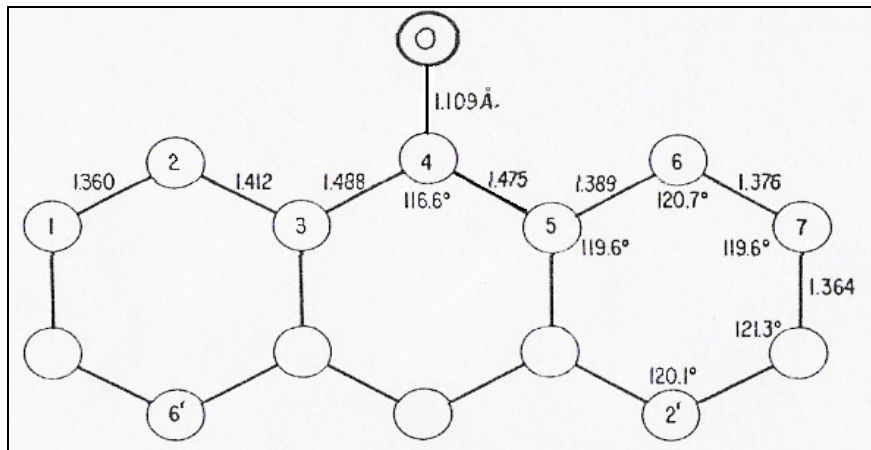


Fig. 1. Bond dimensions in the molecule of anthrone

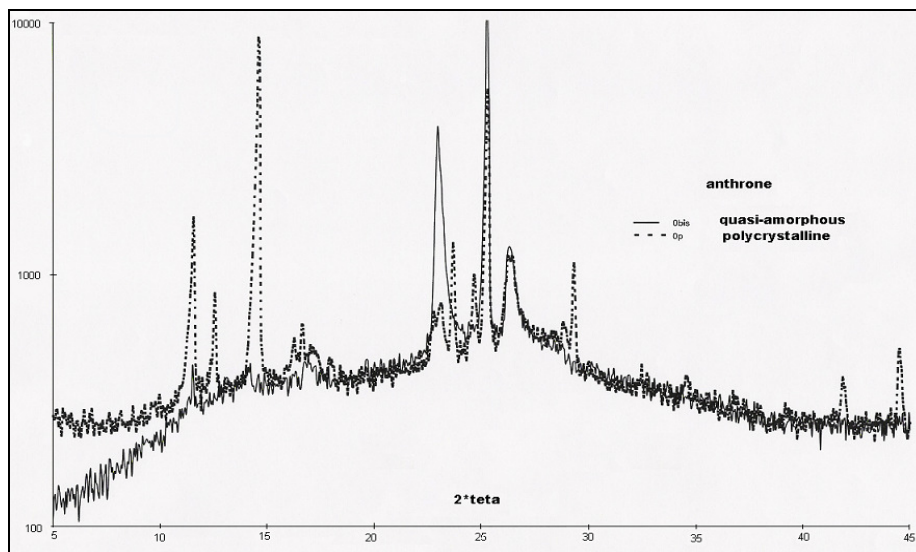


Fig. 2. Diffraction pattern (X-ray) for tested polycrystalline and quasi-amorphous anthrone layers

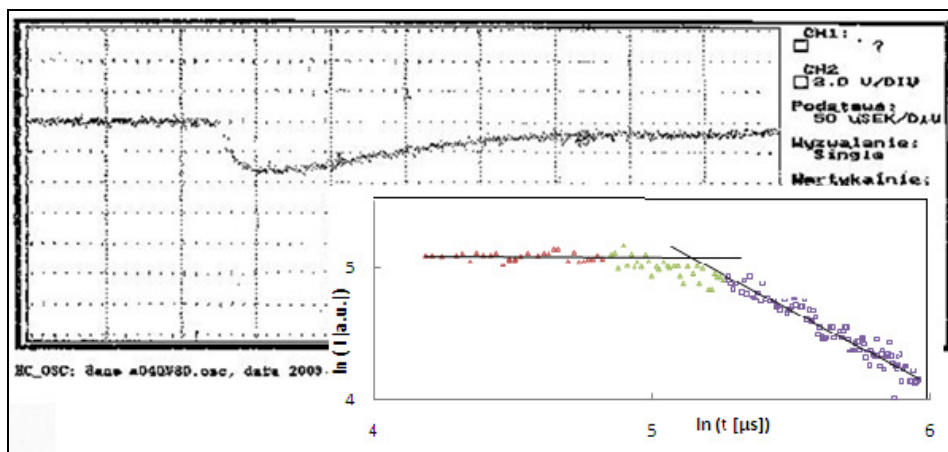


Fig. 3. Typical current pulse for polycrystalline anthrone layers, the insert shows the  $\ln t$  versus  $\ln I$  diagram

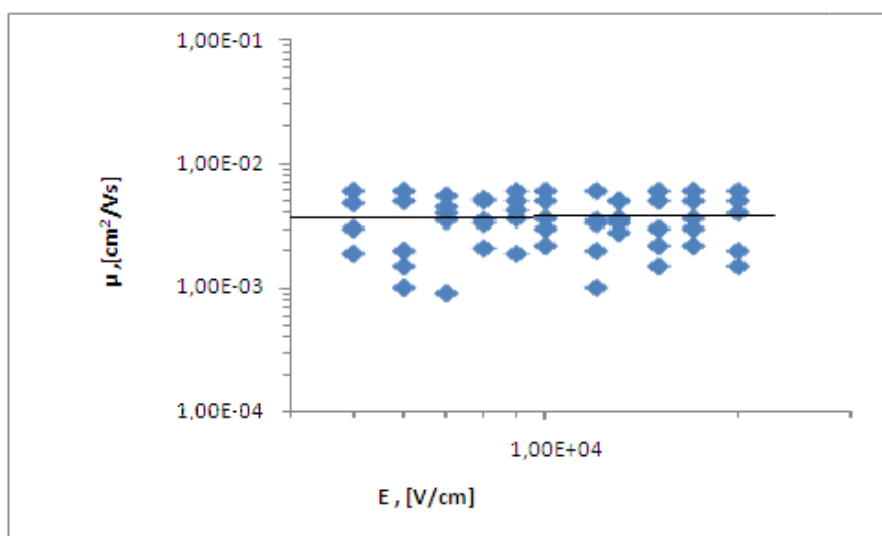


Fig. 4. Electrons drift mobility in polycrystalline anthrone layer

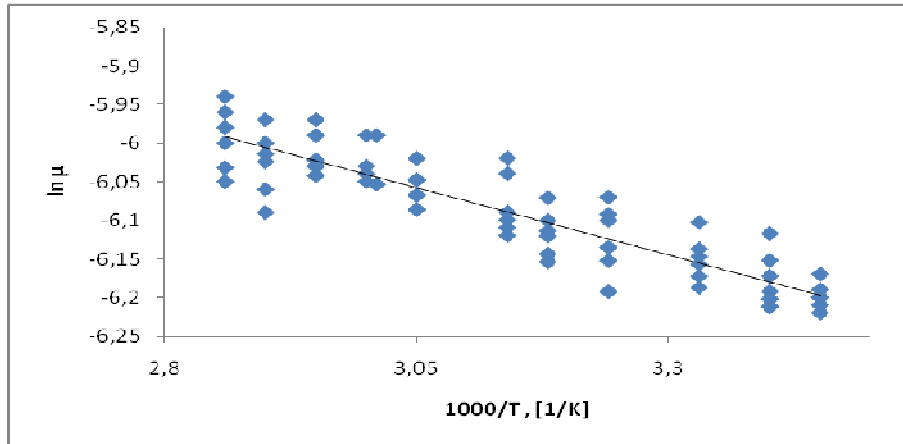


Fig. 5. Temperature dependence of the mobility for polycrystalline anthrone layer

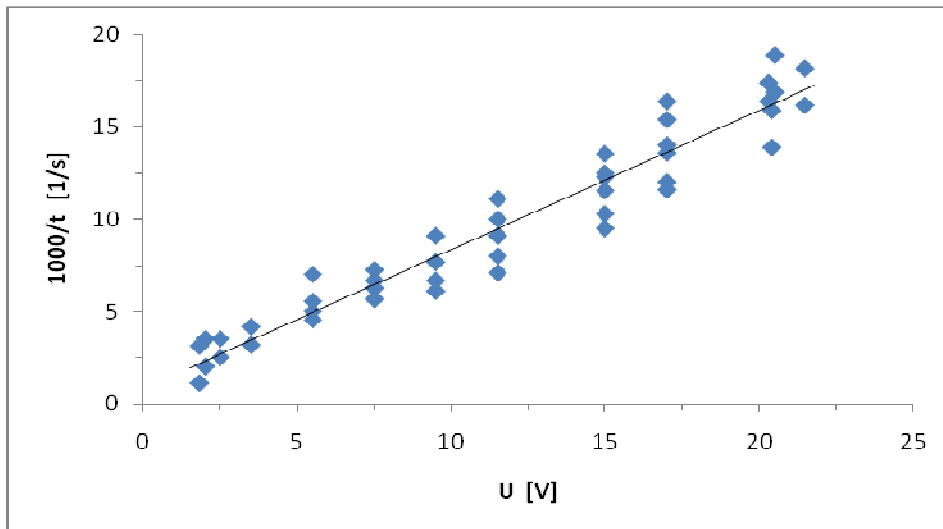


Fig. 6. Inverse time of flight due to the voltage applied to the quasi-amorphous anthrone layer ( $l = 22 \mu\text{m}$ )

The examinations of the electron mobility for the polycrystalline anthrone layers were made in the limits of the electrical field from  $4 \cdot 10^3$  V/cm to  $2 \cdot 10^4$  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 290-350 K. The results of these investigations are shown in the Fig. 5.

For the polycrystalline anthrone layers there were obtained the mobility for electrons in the range  $(1\div 5)\cdot 10^{-3}\text{cm}^2/\text{Vs}$  and the activation energy for mobility on the level of  $kT$ , that is 0,03 eV. For quasi-amorphous anthrone 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. 6.

Generally it can be say that the values of the mobilities for the quasi-amorphous anthrone layers were with a great spread, and were limited in the range  $(0.9\div 6)\cdot 10^{-3}\text{cm}^2/\text{Vs}$ . The values of the activity energy for mobility were determined only in the small range of temperatures, and they were supposed to be in the range of  $kT$ .

### 3. DISCUSSION

For the polycrystalline layers the drift mobility values were in the range  $(1\div 5)\cdot 10^{-3}\text{cm}^2/\text{Vs}$  and activation energy for mobility was in the range near 0,03 eV.

For such obtained values one can make assumption, that the charge carrier transport is possible in the narrow band near the Fermi level.

The hopping mobility for such conditions can be described with the formula:

$$\mu = 1/6(eR^2 / kT)v_{ph} \exp(-2\alpha R)\exp(-\Delta E / kT),$$

where:  $v_{ph}$  – means the phonon frequency,  $\alpha$  – characteristic attenuation coefficient for the wave function. From the Mott – Davies formula we can estimate the mean distance between localized states. Reaching the knowledge on the  $R$  value we can estimate the localized states density as:

$$N(E_F) = (3/4)\pi(1/(R^3\Delta E)),$$

where  $\Delta E$  – means the width of the band considered here as the activation energy.

Taking into account experimentally obtained values for the polycrystalline layers, it was obtained the mean distance between localized states  $R$  as the value in the range from 24 to 12 Å and the density of states  $N(E_F)$  from  $5.7\cdot 10^{21}\text{1/cm}^3\text{eV}$  to  $4.5\cdot 10^{22}\text{1/cm}^3\text{eV}$ .

For the quasi-amorphous layers, where the drift mobility  $\mu$  values were in the range  $(0.9\div 6)\cdot 10^{-3}\text{cm}^2/\text{Vs}$  and the activation energy for mobility were in the order of  $kT$  (i. e. ca. 0.026 eV) one had obtained very similar values. Namely,

the obtained mean distance  $R$  between localized states was in the limits  $24 \div 11 \text{ \AA}$  and the density  $N(E_F)$  of localized states was in the limits from  $6.6 \cdot 10^{21} \text{ 1/cm}^3\text{eV}$  to  $6.8 \cdot 10^{22} \text{ 1/cm}^3\text{eV}$ .

It seems that the obtained density levels are so high, then we ought to think if we really were with the case of the hopping transport in the narrow band near the Fermi level.

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:  $\mu_d(T) \approx \exp(-E_t/kT)$ , where  $E_t$  is the activation energy for hopping [10, 11].

#### 4. CONCLUSIONS

For anthrone layer, which molecules are with the dipole moment, there were determined that:

1. The value of the electron mobility is smaller than  $10^{-2} \text{ cm}^2/\text{Vs}$  and a small worth of the activation energy for mobility on the level of  $kT$ .
2. Taking all of the obtained data into account is impossible to unambiguously to suggest what kind of electron transport we exercised. It appears that the obtained densities of states are so high, then it makes as to think if we are here with the hopping transport in the narrow band near the Fermi level.
3. There is the absence of the effect of the structure of the layer on the electron transport.

#### ACKNOWLEDGEMENTS

Great thanks to dr. B. Marciniak and prof. M. Wieczorek, for preparation of the spectral grade anthrone and for enabling the Roentgen analysis and to Prof. J. Świątek for valuable discussions.



## REFERENCES

- [1] **Yatsenko A.V.**, J. Mol. Model. **9** (2003) 207.
- [2] **Winkler B.**, Kristallogr Z., **214** (1999) 506.
- [3] **Dewar M.J.S., Thiel W.**, Theor. Chim. Acta. **46** (1977) 81.
- [4] **Weber G.**, Z. Naturforsch. **B. 36** (1981) 896.
- [5] **Landolt-Börnstein**, Zahlenwerte und Funktionen aus Naturwissenschaften und Technik, Springer Verlag, Berlin, 1971.
- [6] **Wyckoff R. W. G.**, Crystal Structures vol. 6, Interscience Publishers New York, 1971.
- [7] **Kania S., Kondrasiuk J., Bąk G.W.**, Eur. Phys. J. E. **15** (2004) 439.
- [8] **Kania S.**, Visnyk of Lviv Univ. Series Physical. **40** (2007) 322.
- [9] **Kania S.**, Visnyk of Lviv Univ. Series Physical. **43** (2009) 49.
- [10] **Kania S.**, Sci. Bull. Techn. Univ. Lodz, No. 1082, Physics. **31** (2010) 43.
- [11] **Silins E., Čapek V.**, Organic molecular crystals, AIP Press, New York, 1994.
- [12] **Mycielski, W.E.**, J. Non-Crystalline Solids. **37** (1980) 267.
- [13] **Zahlen R.Z.**, The Physics of Amorphous Solids.. John Wiley and Sons Inc. 1983.
- [14] **Mott N.F., Davies E.A.**, Electronic Processes in Non-Crystalline Materials, Clarendon Press, Oxford. 1971.
- [15] **Kania S., Kondrasiuk J.**, Sci. Bull. Tech. Univ. Lodz, Physics **23** (2003) 25.
- [16] **Kania S.**, Sci. Bull. Tech. Univ. Lodz, Physics **24** (2004) 47.

## DRYFTOWA RUCHLIWOŚĆ ELEKTRONÓW W WARSTWACH ANTRONU

### Streszczenie

Badano proces transportu elektronów w warstwach antronu o różnym stopniu uporządkowania, to jest w warstwach polikrystalicznych i quasi-amorficznych. Pomiaru ruchliwości wykonano metodą TOF. W przypadku antronu, którego cząsteczki posiadają stały moment dipolowy, uzyskano, że prawie nie występuje zależność ruchliwości od stopnia uporządkowania. Dla obu struktur uzyskano wartości ruchliwości mniejsze niż  $10^{-2}$  cm<sup>2</sup>/Vs, z energią aktywacji ruchliwości rzędu  $kT$ . Mimo iż wielkości te przemawiają za transportem hoppingowym, to wydaje się, że otrzymane wartości gęstości stanów są na tyle duże, że należy się zastanowić, czy faktycznie mamy do czynienia z transportem przeskokowym w wąskim paśmie w pobliżu poziomu Fermiego. Poza tym nie obserwujemy wpływu struktury krystalicznej warstw na

wielkość ruchliwości, chyba, że dla polikrystalicznych warstw gęstość stanów jest na tyle duża, że nie należy spodziewać się jej wzrostu. Powyższe skłania nas do stwierdzenia, że nie można jednoznacznie określić, z jakim rodzajem transportu dla elektronów mamy tu do czynienia.