

SYLWESTER KANIA^{1,2}

¹ Institute of Physics, Technical University of Łódź, Wólczańska 219
90-924 Łódź, Poland

² Center of Mathematics and Physics Technical University of Łódź
Al. Politechniki 11, 90-924 Łódź, Poland

ELECTRON DRIFT MOBILITY IN AMORPHOUS ANTHRONE LAYERS

There were investigated the magnitude of the mobility and the type of the mechanism of the electron transport in the amorphous anthrone layers Anthrone ($C_{14}H_{10}O$) is the molecular crystal. The anthrone molecules due to their asymmetry possess permanent dipole moment, $\mu = 1.22 \cdot 10^{-29} \text{Cm}$. The anthrone samples were obtained by evaporation in vacuum under the pressure of the order of 10^{-5} Torr on glass plates with lower substrate temperatures. Structural examination of the obtained anthrone layers was made using X – ray diffraction. In order to attain that one employed an automatic diffractometer DAR. Drift electron mobility for obtained amorphous layers were determined with TOF method. Obtained results shows the almost lack of the mobility dependence due to the magnitude of the disorder, although the other results should be expected. Either obtained mobility value, less than $10^{-2} \text{cm}^2/\text{Vs}$ and activation energy value on the kT level do not permit state unambiguously if we are here with hopping transport mechanism, or with the band transport with participation of the trapping states.

Keywords: amorphous, amorphous anthrone films, electron 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 anthrone, which molecules are with the dipole moment. The second was the antrachinone, which molecules are with the nearly zero dipole moment. As the first there were made the experiments on the carrier mobility for the antrachinone layers and in the second the anthrone layers are examined.

2. EXPERIMENTAL

The structure of anthrone, $C_{14}H_{10}O$, 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):

$A = (15.80 \pm 0.03) \text{Å}$, $b = (3.998 \pm 0.005) \text{Å}$, $c = (7.86 \pm 0.16) \text{Å}$ and $\beta = 101^{\circ} 40'$ [5, 6].

The space group $C2h5(P21/a)$ places its atoms in the positions: $\pm(xyz; x+1/2, 1/2 - y, z)$ with oxygens distributed statistically over half these positions. The parameters are those of the Table 1.

Planar, with asymmetrical molecules have the bond dimensions shown in the Fig. 1. The anthrone molecule possesses 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 for amorphous layers was 150-165 K with a proper evaporation rate. Structural examinations obtained anthrone layers were made using X – ray diffraction.

Table 1

Parameters of atoms in anthrone

Atom	x	y	z
C(1)	0.1358	0.3934	0.3904
C(2)	0.0550	0.2641	0.3404
C(3)	0.0278	0.1333	0.1714
C(4)	0.0605	0.0107	- 0.1265
C(5)	0.0847	0.1463	0.0576
C(6)	0.1666	0.2816	0.1133
C(7)	0.1915	0.4077	0.2787
$\frac{1}{2}$ O	0.1052	0.0238	- 0.2118

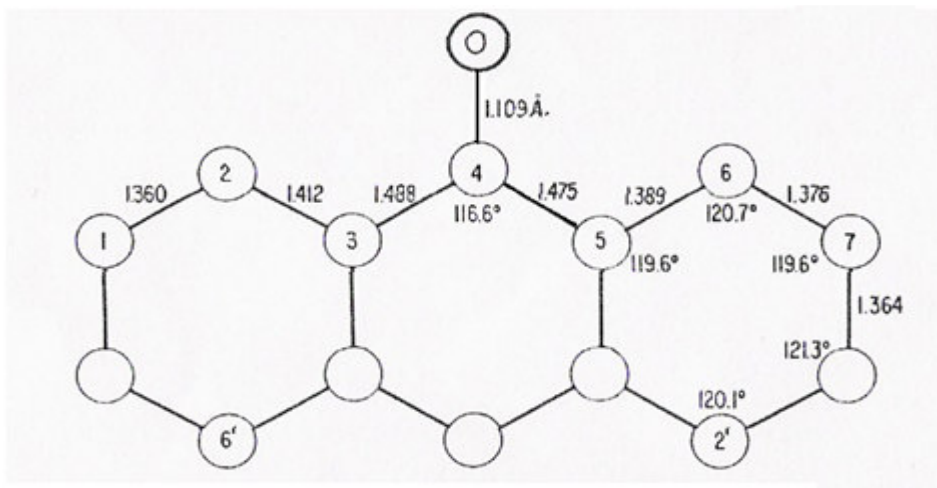


Fig. 1. Bond dimensions in the molecule of anthrone

For this purpose the automatic diffractometer DAR was employed. Diffraction examinations were made in the 2θ range from 5° to 80° with measuring step $0,05^\circ$.

Typical diffraction patterns for tested amorphous films are described with Fig 2.

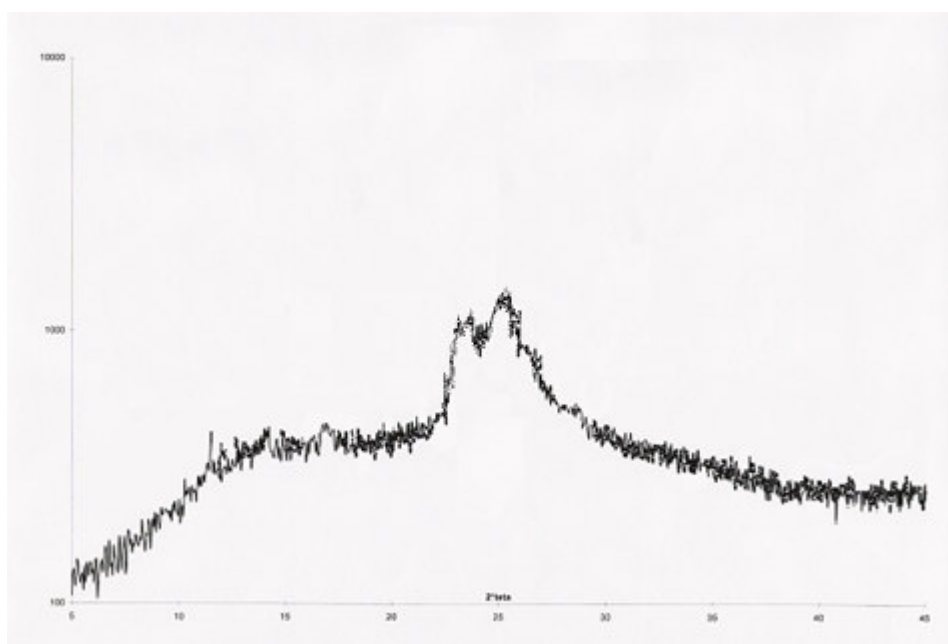


Fig. 2. Diffraction pattern (X ray) for tested amorphous anthrone layers

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. The system is completely described in [7-10, 15, 16].

Typical current pulse obtained for the amorphouse anthrone layers is presented in Fig. 3.

The examinations of the electron mobility for the amorphous anthrone layers were made in the limits of the electrical field from $5 \cdot 10^3$ V/cm to $6 \cdot 10^4$ 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 290-310 K. The results of

these investigations are shown in the Fig. 5. For the amorphous anthrone layers there were obtained the mobility for electrons in the range $(0.6\div 3)\cdot 10^{-3} \text{ cm}^2/\text{Vs}$ and the activation energy for mobility on the level of kT , that is 0,026 eV.

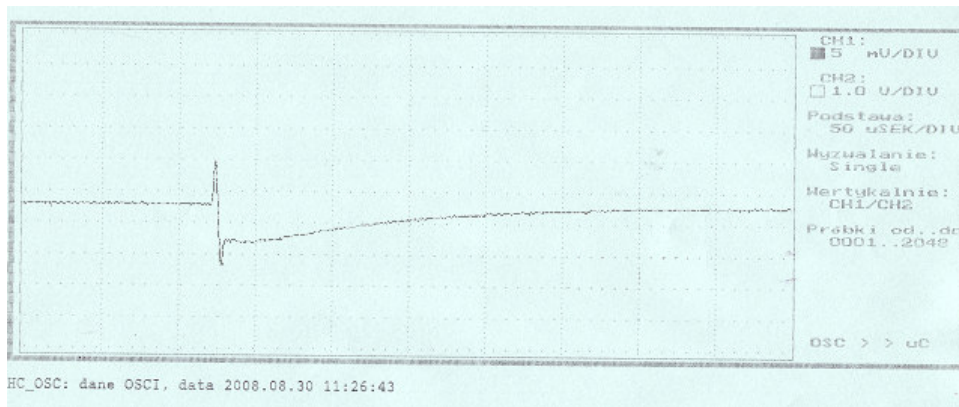


Fig. 3. Typical current pulse for amorphous anthrone layers

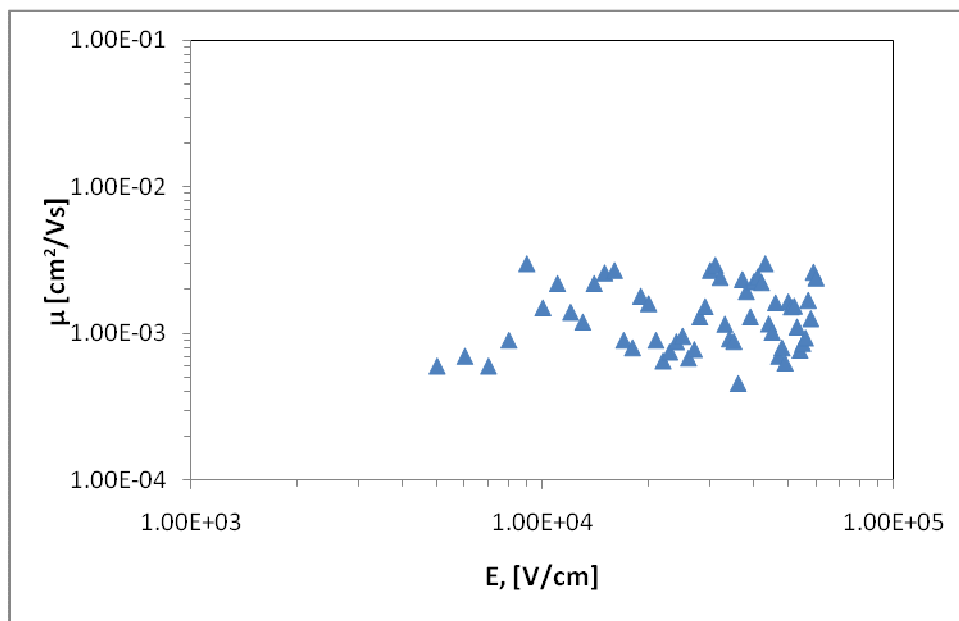


Fig. 4. Electron drift mobility in amorphous anthrone layer

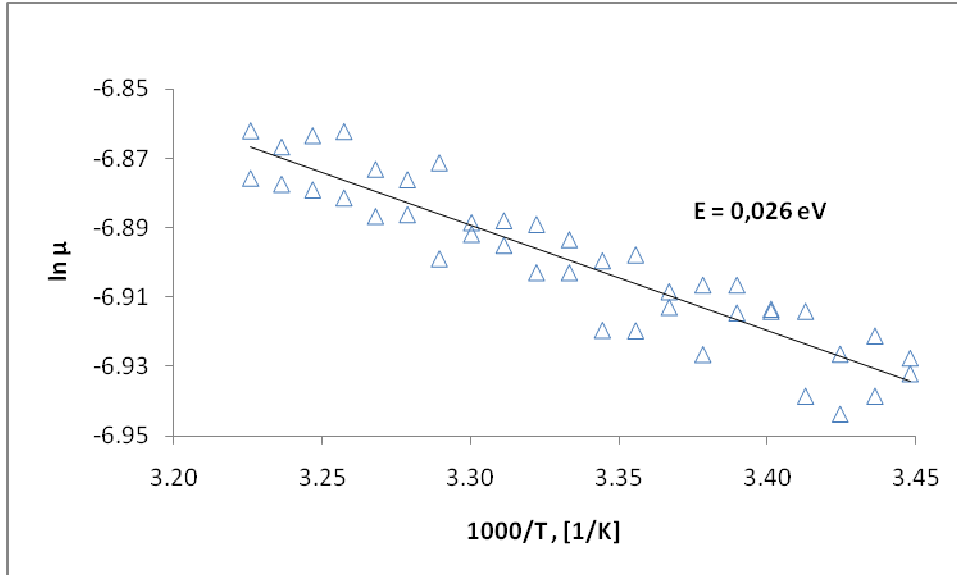


Fig. 5. Temperature dependence of the mobility for amorphous anthrone layer

For the amorphous anthrone layers there were the wide spread of the mobility values, what is seen in the Fig. 4. The same was for the activation energy values for mobility, despite this the trend of the dependence was the same as for polycrystalline layers.

Generally it was obtained that the values of the mobility for the amorphous anthrone layers were with a great spread, and they were limited in the range $(0.6 \div 3) \cdot 10^{-3} \text{ cm}^2/\text{Vs}$. The value of the activation energy for mobility was determined only in the small range of temperatures, and its value can be supposed in the range of kT . For the transport in polycrystalline materials 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]. Similarity of both descriptions make impossible, in the scope of this article, to judge which mechanism dominates.

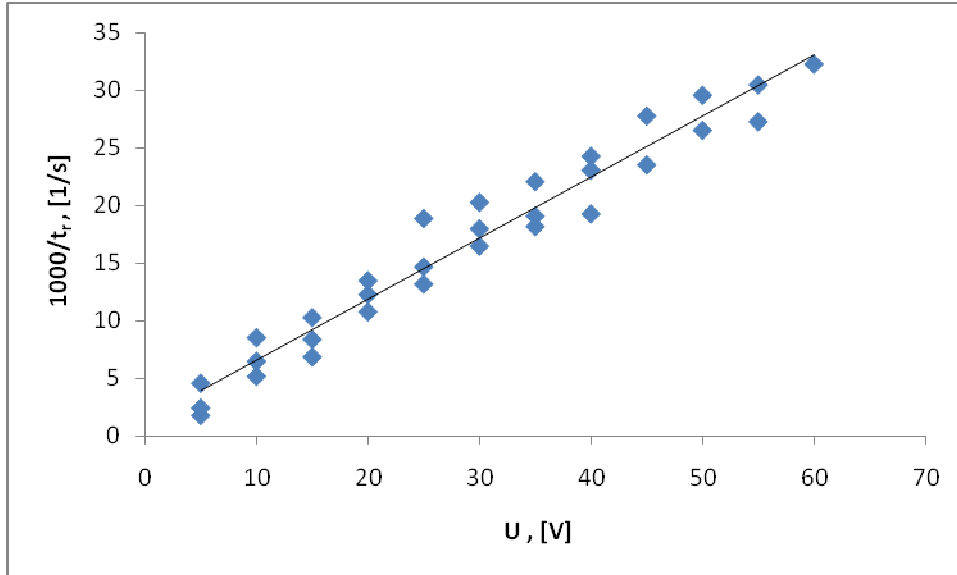


Fig. 6. Inverse time of flight due to the voltage applied to the amorphous anthrone layer, for the exemplary layer, $L \approx 20 \mu\text{m}$

If it is accepted the conclusion, that the dominant mechanism is hopping mechanism, then for the mobility value of $0.6 \cdot 10^{-3} \text{ cm}^2/\text{Vs}$ and the activation energy of the order kT the mean distance between localized states should be $R \approx 24 \text{ \AA}$ and the density of localized states in proximity of the Fermi level $N(E_F) \approx 6.5 \cdot 10^{21} \text{ cm}^{-3} \text{ eV}^{-1}$. Those quantities can be accepted. Although for the mobility value of $3 \cdot 10^{-3} \text{ cm}^2/\text{Vs}$ the mean distance between localised states must be $R \approx 9 \text{ \AA}$ and $N(E_F) \approx 1.2 \cdot 10^{22} \text{ cm}^{-3} \text{ eV}^{-1}$, both this values are rather typical for the band model.

3. 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 value of the activation energy for mobility is on the level of kT ,
2. the hopping transport [12, 14] or the band transport [13] is with participation of the traps.

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 prof J. Świątek for valuable discussions.

REFERENCES

- [1] **Dovesi R. J.**, J Chem. Phys., Vol. **92**, **12** (1990). 7402.
- [2] **Winkler B.**, Z. Kristallogr., Vol. **214** (1999) 506.
- [3] **Dewar M.J.S., Thiel W.A.**, Theor. Chim. Acta., Vol. **46**, **2** (1977) 81.
- [4] **Weber G.**, Z. Naturforsch. B., Vol. **36**, **7** (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. Vol. **40** (2007) 322.
- [9] **Kania S.**, Sci. Bull. Łódź Technical University. s. Physics. Vol. **22** (2002) 31.
- [10] **Kania S.**, Sci. Bull. of Łódź Technical University, s. Physics., Vol. **24** (2004) 47.
- [11] **Silinsh E., Čapek V.**, Organic molecular crystals, AIP Press, New York, 1994.
- [12] **Mycielski W. J.** Non-Crystalline Solids., Vol. **37** (1980) 267.
- [13] **Zahlen R.**, 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. Scientific Bull. of Technical Univ. of Łódź. s. Physics vol. **23** (2003) 25.
- [16] **Kania S.**, Scientific Bull. of Technical Univ. of Łódź. s. Physics., Vol. **24** (2004) 47.

RUCHLIWOŚĆ DRYFTOWA ELEKTRONÓW W AMORFICZNYCH WARSTWACH ANTRONU

Streszczenie

Badano proces transportu elektronów w warstwach. Uzyskane wyniki nie przesądzają jednoznacznie z jakim rodzajem transportu mamy do czynienia. Uzyskane wyniki mogą sugerować występowanie zarówno transportu hoppingowego, jak i transportu w paśmie z udziałem pułapek.