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HOLE DRIFT MOBILITY IN ANTHRONE LAYERS

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There were investigated the magnitude of the mobility and the type of the mechanism of the hole transport in the anthrone layers with a different grade of the structural order, namely in polycrystalline and quasi-amorphous layers. Anthrone ($C_{14}H_{10}O$) is the molecular crystal with the cell parameters: $a = (15,80\pm0,03)$Å, $b = (3,998\pm0,005)$Å, $c = (7,86\pm0,16)$Å   and $\beta = 101°40'$. The anthrone molecules due to theirs asymmetry posses permanent dipole moment, $\mu = 1,22\cdot10^{-29}$Cm. 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 anthron layers was made using X – ray diffraction. In order to attain that one employed an automatic diffractometer DAR. Diffraction examinations were made in the 2θ range from 5º to 80º with measuring step 0,05º. Drift hole mobility for obtained polycrystalline and quasi-amorphous layers were determined with TOF method. Experimental set up and the method for determination of the mobility are described in the earlier works. 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 then 10^{-2} cm^2/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.

Key words: quasi-amorphous, polycrystalline anthrone films, hole drift mobility, carrier transport.

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 anthron, 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.

The structure of anthrone, $C_{14}H_{10}O_2$, has been repeatedly investigated, most recently at several temperatures between 170 and 20°C. Its crystals are monoclinic with bimolecular unit of the dimensions (in room temperature):

a= (15,80±0,03)Å , b= (3,998±0,005)Å , c= (7,86±0,16)Å and β= 101° 40′ [5, 6].

The space group C_{2h}^5(P2$_1$/a) places its atoms in the positions: ±(xyz; x+$^1/_2$, $^1/_2$−y, z) with oxygens distributed statistically over half these positions. The parameters are those of the table 1.

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
½O	0,1052	0,0238	- 0,2118

Planar, with asymmetrical molecules have the bond dimensions shown in the fig 1. The anthrone molecule posses a natural dipole moment measured in benzene 3,66 D (1,22·10^{-29} Cm) [6].
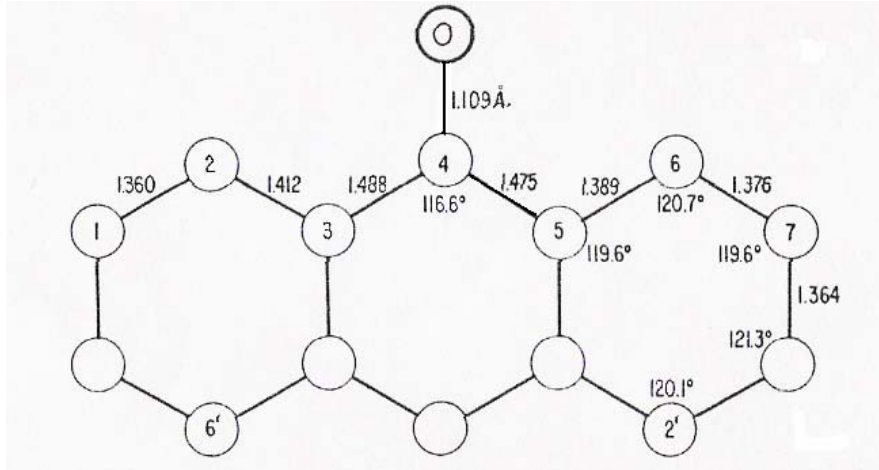
Fig. 1. Bond dimensions in the molecule of anthrone

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 obtained anthrone layers were made using X – ray diffraction. For this purpose the automatic diffractometer DAR was employed. Diffraction examinations were made in the 2θ range from 5º to 80º with measuring step 0,05º.

Typical diffraction patterns for tested polycrystalline and quasi-amorphous films are both described with fig. 2.
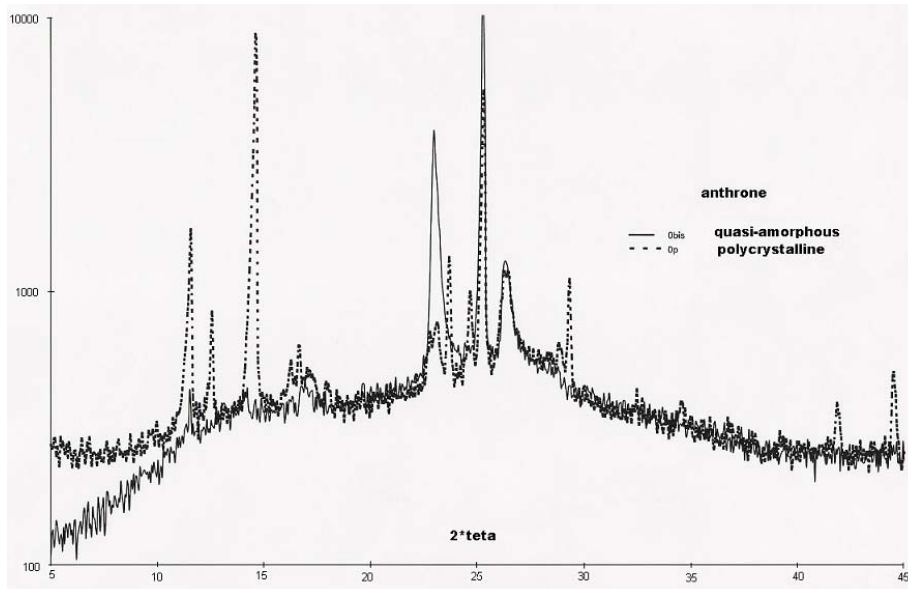

Fig. 2. Diffraction pattern (X ray) for tested polycrystalline and quasi-amorphous anthrone layers

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 [7 – 10, 15, 16].

Typical current pulse obtained for the polycrystalline anthrone layers is presented in fig. 3.
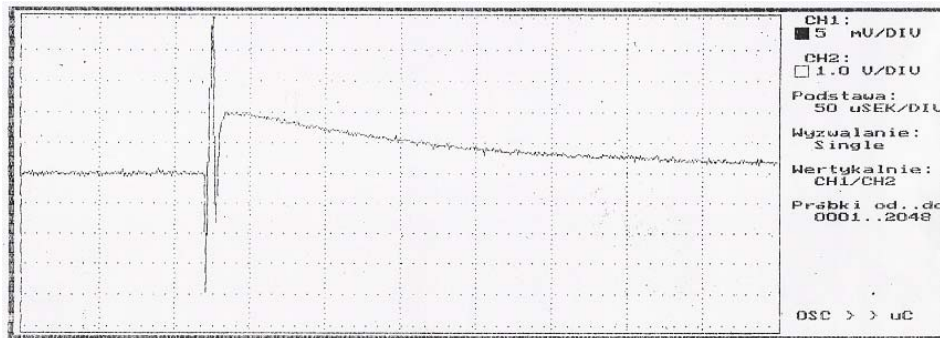

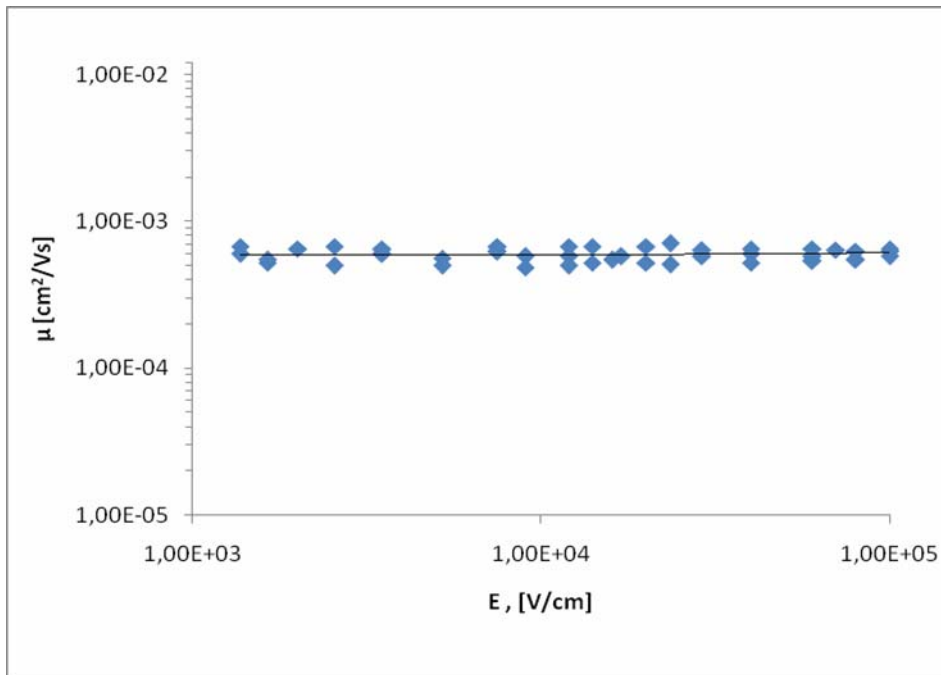Fig. 3. Typical current pulse for polycrystalline anthrone layers

Fig. 4. Hole drift mobility in polycrystalline anthrone layer

The examinations of the hole mobility for the polycrystalline anthrone layers were made in the limits of the electrical field from $1·10^3$ to $1·10^5$ 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. 5. For the polycrystalline anthrone layers there were obtained the mobility for holes in the range $(6±2)·10^{-4}$ cm^2/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).
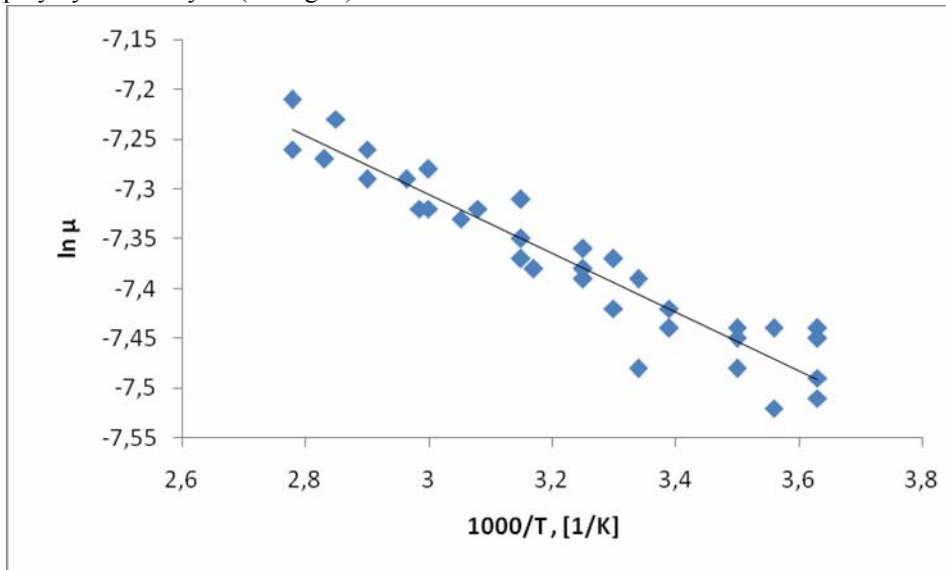

Fig. 5. Temperature dependence of the mobility for polycrystalline anthrone layer

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 mobility for the quasi-amorphous anthrone layers were with a great spread, and were limited in the range $(3 – 7)·10^{-4}$ cm^2/Vs. 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 $\mu_d(T) = a\ T^{-n}·b\ \exp(-E_t/kT)$, 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].
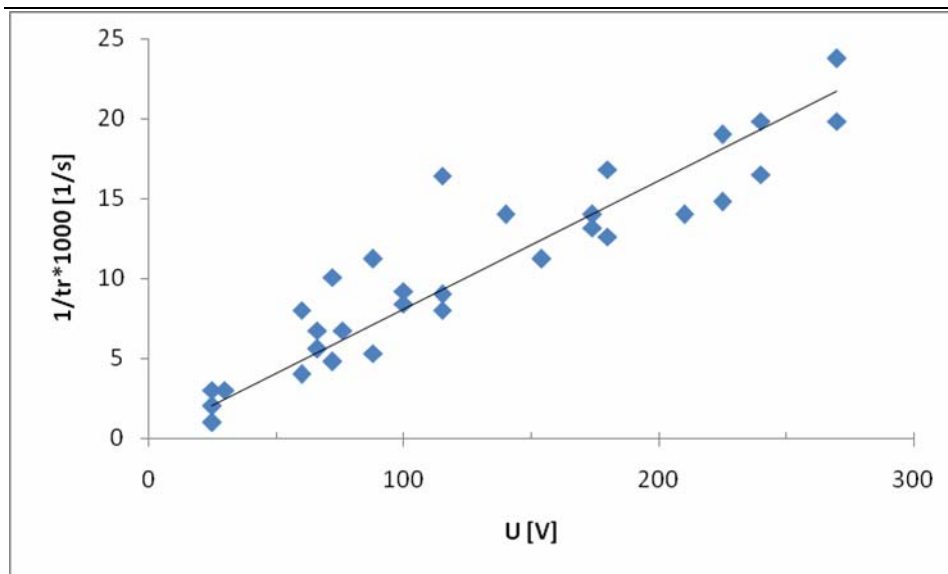
Fig. 6. Inverse time of flight due to the voltage applied to the quasi-amorphous anthrone layer

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

1. the value of the hole mobility is smaller then 10^{-3} cm^2/Vs and a small worth of the activation energy for mobility on the level of kT;

2. the hopping transport [12, 14] or the band transport [13] 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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1. *Dovesi R. J.* Ab initio approach to molecular crystals: A periodic Hartree–Fock study of crystalline urea source // J. Chem. Phys. 1990. Vol. 92. N. 12. P. 7402–7411.
2. *Winkler B.* An introduction to computational crystallography // Z. Kristallogr. 1999. Vol. 214. P. 506 – 527.
3. *Dewar M.J.S., Thiel W.* A semiempirical model for the two-center repulsion integrals in the NDDO approximation // Theor. Chim. Acta. 1977. Vol. 46. N 2. P. 81.
4. *Weber G.* the structure of a 2:1 host guest complex between p-nitroaniline and 18-crown-6 // Z. Naturforsch. B. 1981. Vol. 36. N 7. P. 896–897.
5. *Landolt-Börnstein.* Zahlenwerte und Funktionen aus Naturwissenschaften und Technik, Springer Verlag, Berlin, 1971.
6. *Wyckoff R.W.G.* Crystal Stuctures. Interscience Publishers New York, 1971. Vol. 6.

7. *Kania S., Kondrasiuk J., Bąk G.W.,* Influence of ambient atmosphere on charge transport in polycrystalline thin films of three simple aromatic hydrocarbons // Eur. Phys. J. E. 2004. N 15. P. 439–442.

8. *Kania S.* Charge carrier transport in the tetracene layers with a different structural order // Visnyk of Lviv. Univ. Ser. Physical. 2007. Vol. 40. P. 322–336.

9. *Kania S.* An effect of activation on electrical properties of aromatic hydrocarbons // Sci. Bull. Łódź Technical Univ. Ser. Physics. 2002. Vol. 22. P. 31–37.

10. *Kania S.* The magnitude of the order and the hole transport in the tetracene films // Sci. Bull. of Łódź Technic. Univ. Ser. Physics. 2004. Vol. 24. P. 47–59.

11. *Silinsh E., Čapek V.* Organic molecular crystals, AIP Press, New York, 1994.

12. *Mycielski W.* Evidence of hopping conduction among localized states in disordered systems of simple aromatic compounds // J. Non–Cryst. Solids. 1980. Vol. 37. 267 p.

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–Cryst. Materials. Clarendon Press, Oxford. 1971.

15. *Kania S., Kondrasiuk.* Drift hole mobility in the amorphous tetracene films // J. Scientific Bull. of Technic. Univ. of Łódź. Ser. Physics. 2003. Vol. 23. 25 p.

16. *Kania S.* The magnitude of the order and the hole transport in the tetracene films // Scientific Bull. of Technic. Univ. of Łódź. Ser. Physics. 2004. Vol. 24. P. 47–59.

ДРЕЙФОВА РУХЛИВІСТЬ ДІРОК В АНТРОНОВИХ ШАРАХ

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Досліджено механізм рухливості дірок в андронових шарах з різним ступенем структурної досконалості, а саме − в полікристалічних і квазіаморфних шарах. Антрон ($C_{14}H_{10}O$) − молекулярний кристал з параметрами гратки: $a = (15{,}80{\pm}0{,}03)$ Å, $b = (3{,}998{\pm}0{,}005)$ Å , $c = (7{,}86{\pm}0{,}16)$ Å і $\beta = 101°40´$. Антронові зразки одержані шляхом випаровування у вакуумі під тиском 10-5 Торр. Структуру отриманих шарів досліджували методом рентгенівської дифракції. Дрейфову рухливість дірок для полікристалічних та квазіаморфних шарів досліджено методом TOF. Отримані результати засвідчують відсутність залежності рухливості від величини розпорядкування.

Ключові слова: квазіаморфні, полікристалічні антронові плівки, рухливість дірок, перенесення носіїв заряду.

ДРЕЙФОВАЯ ПОДВИЖНОСТЬ ДЫРОК В АНТРОНОВЫХ СЛОЯХ

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Исследовано механизм подвижности дырок в андроновых слоях сразной степенью структурного совершенства, а именно – в поликристаллических и квазиаморфных слоях. Антрон ($C_{14}H_{10}O$) – молекулярный кристалл с параметрами решетки: a = (15,80±0,03) Å, b = (3,998±0,005) Å, c = (7,86±0,16) Å и β = $101^0 140^{'}$. Антроновые образцы получены путем испарения в вакууме под давлением 10–5 Торр. Структуру полученных слоев исследовали методом рентгеновской дифракции. Дрейфовую подвижность дырок для поликристаллических и квазиаморфных слоев исследовано методом TOF. Полученные результаты указывают на отсутствие зависимости подвижности от величины разупорядочения.

Ключевые слова: квазиаморфные, поликристаллические антроновые пленки, подвижность дырок, перенос носителей заряда.