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ELECTRON DRIFT MOBILITY IN AMORPHOUS ANTHRAHINONE LAYERS

There were investigated the magnitude of the mobility and the type of the mechanism of the electron transport in the amorphous antrachinone layers. Antrachinone ($C_{14}H_8O_2$) is the molecular crystal. The antrachinone molecules are planar, centrosymmetric and posses permanent dipole moment practically equal zero. The antrachinone layers were obtained by evaporation in vacuum under the pressure of the order of 10^{-5} Torr on glass plates with reduced substrate temperatures. Structural examination of the obtained antrachinone 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 mobility value, were less then 10^{-3} cm^2/Vs and activation energy value was on the kT level.

Keywords: amorphous, amorphous antrachinone films, electron drift mobility, carrier transport.

1. INTRODUCTION

The precise measurements show that thin film organic crystals are technologically in the electronic meaning very attractive materials.

The properties related to the electronic structure of these materials like photoconductivity, light absorption, non-linear polarizability etc. are the source of theirs usefulness. 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 are

very difficult and sometimes are 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 [17]. The second was the antrachinone, which molecules are with the nearly zero dipole moment.

2. EXPERIMENTAL

The structure of antrachinone, $C_{14}H_8O_2$, 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):

$a = (15.810 \pm 0.015) \text{Å}$, $b = (3.942 \pm 0.005) \text{Å}$, $c = (7.865 \pm 0.010) \text{Å}$ and $\beta = 102^{\circ} 43'$ [5, 6].

The space group $C_{2h}5(P2_1/a)$ places its atoms in the positions: $\pm(xyz; x + 1/2, 1/2 - y, z)$.

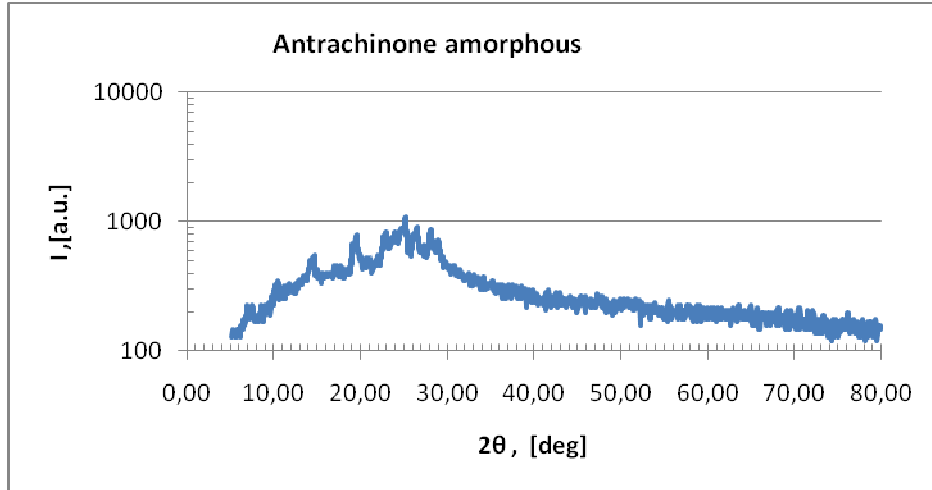


Fig. 2. Diffraction pattern (X-ray) for tested amorphous anthracinone layers

Typical current pulse obtained for the amorphous anthracinone layers is presented in Fig. 3.

Based on obtained current pulses there were determined the time of flight for electrons what enabled for them determination of the value of the drift mobility (exemplary dependence was presented in the Fig. 4 for examined layer in the dependence on voltage).

The examinations of the electron mobility for the amorphous anthracinone layers were made in the limits of the electrical field from $1 \cdot 10^3$ V/cm to $2 \cdot 10^4$ V/cm. The investigations were made in the room temperature and the results are presented in Fig. 5. For the amorphous anthracinone layers there were obtained the mobility for electrons in the range $(0.4 \div 6) \cdot 10^{-4}$ cm²/Vs and the activation energy for mobility on the level of kT.

For the amorphous anthracinone layers there were the wide spread of the mobility values, what is seen in the Fig. 5. The same was for the activation energy values for mobility, despite this fact 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 anthracinone layers were with a great spread, and they were limited in the range $(0.4-6) \cdot 10^{-4}$ cm²/Vs. The value of the activation energy for mobility was determined only in the small range of temperatures, and its value can be

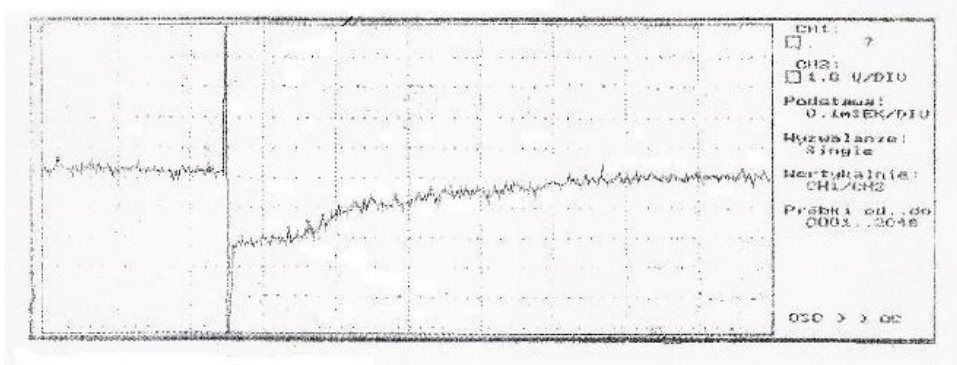


Fig. 3. Typical current pulse for amorphous anthracinone layers, voltage $U = 30$ V, width of the film $L = 18$ μm

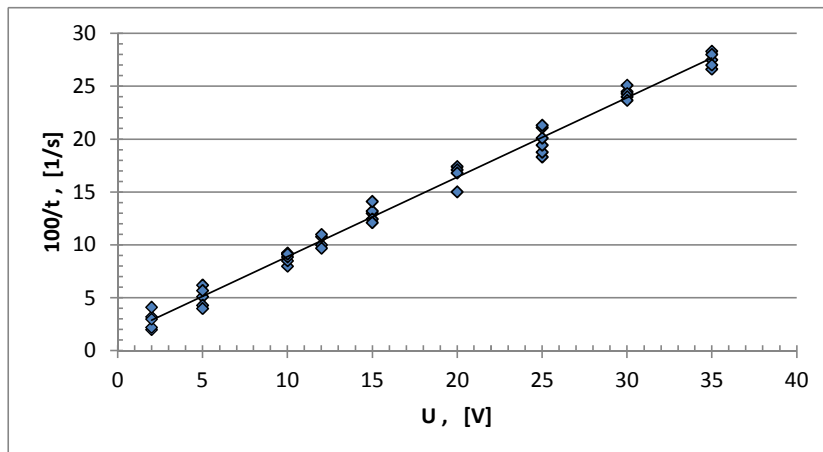


Fig. 4. Inverse time of flight due to the voltage applied to the amorphous anthracinone layer, for the exemplary layer, $L \approx 18$ μm

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: $\mu_d(T) = a T^{-n} b \exp(-E_t/kT)$, 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.

Nevertheless, it seems that there is accepted conclusion that the hopping transport dominant mechanism is.

The drift mobility in the Mott-Davies model is given by:

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

where; R – is the average distance between localized states, e – is electron charge, v_{ph} – is the phonon frequency, α – is decay of the localized state wave function, ΔE – is the width of the narrow band localized states taking part in the charge transport. Usually α^{-1} is burdened with some uncertainty. Using the expression for carrier mobility and geometric formula for density of states:

$$N(E_F) = (3/4\pi)(1/R^3\Delta E) \quad (2)$$

One can estimate the average distance between the localized states and the density of localized states at Fermi level. The spread of mobility values for charge carriers (both electrons and holes) might result from structural changes in layers during conducting the observation. Therefore achieved results should be further investigated, Basing on the expressions (1) and (2) we might estimate average values of the distances for localized states $N(E_F)$ near Fermi level.

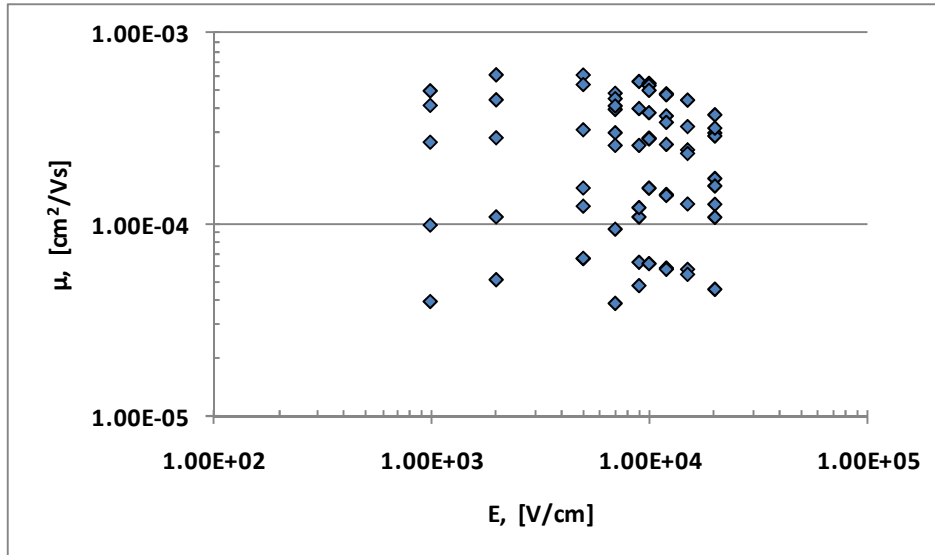


Fig. 5. Electron drift mobility in amorphous anthracinone layer

If it is made an assumption, that the dominant mechanism is hopping mechanism, then for the mobility value of $0.4 \cdot 10^{-4} \text{ cm}^2/\text{Vs}$ and the activation energy of the order kT the mean distance between localized states should have be $R \approx 40 \text{ \AA}$ and the density of localized states in proximity of the Fermi level should have be $N(E_F) \approx 5,7 \cdot 10^{20} \text{ cm}^{-3} \text{ eV}^{-1}$. Those quantities can be accepted. And for the mobility value of $6 \cdot 10^{-4} \text{ cm}^2/\text{Vs}$ the mean distance between localized states must be $R \approx 24 \text{ \AA}$ and $N(E_F) \approx 6,5 \cdot 10^{21} \text{ cm}^{-3} \text{ eV}^{-1}$. Both of these values can be accepted in the scope of hopping model.

3. CONCLUSIONS

For anthracinone layer, which molecules are without any dipole moment, there were determined that:

1. the value of the electron mobility is smaller then $10^{-3} \text{ cm}^2/\text{Vs}$ and a value of the activation energy for mobility is on the level of kT ,
2. the layers were highly unstabilized in theirs electric properties, and this was appeared in experiment as a high spread of the mobility values measured for the tested layer,
3. the hopping transport [12, 14] is more probable then the band transport [13] with participation of the traps.

ACKNOWLEDGEMENTS

Great thanks to dr B. Marciniak and prof. M. Wiczorek for preparation of the spectral grade anthracinone and for enabling the roentgen analysis and prof J. Świątek for valuable discussions.

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RUCHLIWOŚĆ DRYFTOWA ELEKTRONÓW W AMORFICZNYCH WARSTWACH ANTRACHINONU

Streszczenie

Badano proces transportu elektronów w amorficznych warstwach antrachinonu. Uzyskane wyniki nie przesądzają jednoznacznie, z jakim rodzajem transportu mamy do czynienia.

Niemniej uzyskane wyniki mogą sugerować występowanie również transportu hoppingowego, który wydaje się bardziej prawdopodobny, niż transport w pasmie z udziałem pułapek.