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MECHANISMS OF CURRENT FLOW IN IODINE-DOPED POLYMETHYL METHACRYLATE

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Abstract: The mechanisms of current flow in polymethyl methacrylate (PMMA) doped with molecular iodine were investigated. Analysis of the current-voltage characteristics revealed a sequential change in conductivity modes with increasing voltage: ohmic mode, space-limited current mode (SCLC), and trap-limited current mode (TCLC). It was established that these modes are associated with the formation of polyiodide complexes in the polymer matrix, which create trap states of varying depths in the band gap between the HOMO and LUMO levels. The obtained results demonstrate a fundamental difference between the charge-transport mechanisms in iodine-doped PMMA and classical band transport in crystalline silicon.

Keywords: PMMA, iodine doping, polyiodides, traps, SCLC, TCLC, Poole-Frenkel effect, current-voltage characteristics.

YOD BILAN DOPINGLANGAN POLIMETILMETAKRILATDA TOK OQIMI MEXANIZMLARI

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Annotatsiya: Maqolada molekulyar yod bilan dopinglangan polimetilmetakrilat (PMMA)da tok oqimi mexanizmlari o‘rganilgan. Volt-amper tavsiflari tahlili kuchlanish ortishi bilan o‘tkazuvchanlik rejimlarining ketma-ket almashinishini ko‘rsatdi: omik rejim, fazoviy zaryad bilan cheklangan tok (SCLC) rejimi va tuzoqlar bilan cheklangan tok (TCLC) rejimi. Ushbu rejimlar polimer matritsada poliiyodid komplekslarining hosil bo‘lishi bilan bog‘liq bo‘lib, ular HOMO va LUMO darajalari orasidagi taqiqlangan zonada turli chuqurlikdagi tuzoq holatlarini vujudga keltiradi. Olingan natijalar yod bilan dopinglangan PMMAda zaryad tashilish mexanizmlari kristall kremniydagi klassik zonaviy tashilishdan tubdan farqlanishini ko‘rsatadi.

Kalit so‘zlar: PMMA, yod bilan dopinglash, poliiyodidlar, tuzoqlar, SCLC, TCLC, Pul-Frenskel effekti, volt-amper tavsiflari.

МЕХАНИЗМЫ ПРОТЕКАНИЯ ТОКА В ПОЛИМЕТИЛМЕТАКРИЛАТЕ, ЛЕГИРОВАННОМ ЙОДОМ

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Аннотация: В статье исследованы механизмы протекания тока в полиметилметакрилате (PMMA), легированном молекулярным йодом. Анализ вольт-амперных характеристик показал последовательную смену режимов проводимости при увеличении напряжения: омический режим, режим тока, ограниченного пространственным зарядом (SCLC), и режим тока, ограниченного ловушками (TCLC). Установлено, что эти режимы связаны с образованием в полимерной матрице полиодидных комплексов, создающих ловушечные состояния различной глубины в запрещённой зоне между уровнями HOMO и LUMO. Полученные результаты показывают принципиальное отличие механизмов переноса заряда в PMMA, легированном йодом, от классического зонного переноса в кристаллическом кремнии.

Ключевые слова: PMMA, легирование йодом, полиодиды, ловушки, SCLC, TCLC, эффект Пула–Френкеля, вольт-амперные характеристики.

INTRODUCTION

Polymer dielectrics and organic materials have attracted considerable attention in recent decades due to the potential to control their electrical properties through doping, structural modification, and composite formation. Unlike crystalline semiconductors such as silicon, where charge transport is determined by the band structure and concentration of donor and acceptor impurities, injection and trapping conduction mechanisms predominate in polymers [1-5].

Polymethyl methacrylate (PMMA) is a typical wide-bandgap dielectric with an amorphous structure and high dielectric strength. The introduction of molecular iodine into PMMA leads to the formation of polyiodide complexes, which can significantly alter the nature of electrical conductivity. Literature shows that iodine doping in polymer matrices results in the formation of ions I^-, I_3^- и I_5^-,that create localized energy levels (traps) in the bandgap and determine the nonlinear shape of the current-voltage characteristics.

The aim of this work is a model analysis of the current flow mechanisms in iodine-doped PMMA, with the identification of ohmic conductivity, space-limited current (SCLC) and trap - limited current (TCLC) modes, as well as the interpretation of these modes in terms of the dominance of different polyiodide forms.

MATERIALS AND METHODS

Obtaining samples. PMMA samples were produced as nanofibers by electrospinning, followed by doping with molecular iodine. Doping was accomplished by introducing an iodine alcohol solution into the PMMA solution, followed by heat treatment at 50-60 $^\circ$C for 60 minutes. After heat treatment, the samples were kept at room temperature for at least 12-24 hours to stabilize the iodine distribution.

The iodine concentration was selected in the range of 0.6–1.2 wt.%, which made it possible to observe all characteristic current flow modes.

Geometry and electrical contacts. The electrodes were formed from a composite of graphite and liquid glass. The distance between the electrodes was L = 2-4 mm, and the contact area was approximately $S \approx 10 - 20 mm^2$. This geometry allowed current measurements in the nanoampere to milliampere range at voltages up to 50 V.

Measurement technique. The volt-ampere characteristics were measured at room temperature using a constant voltage source (batteries connected in series) and a digital multimeter in current measurement mode. The voltage was changed in steps:

0–10 V in 0.5 V steps and 10–50 V in 2 V steps. At each point, a pause of 5-10 seconds was maintained to allow the charges to relax. To analyze the conductivity mechanisms, the data were presented in coordinates$lgI - lgV$.

RESULTS

Volt-ampere characteristics. A typical I–V characteristic of iodine-doped PMMA exhibits a pronounced nonlinear shape. The coordinates $lgI - lgV$exhibit several linear sections with varying slopes, indicating a change in the current flow mechanism with increasing voltage.

In the region of low stresses, the slope of the dependence is close to one, $(n \approx 1)$,at medium stresses – to two $(n \approx 2)$, and in the region of high stresses, the slope increases to values $n \approx 4$.(Fig.)

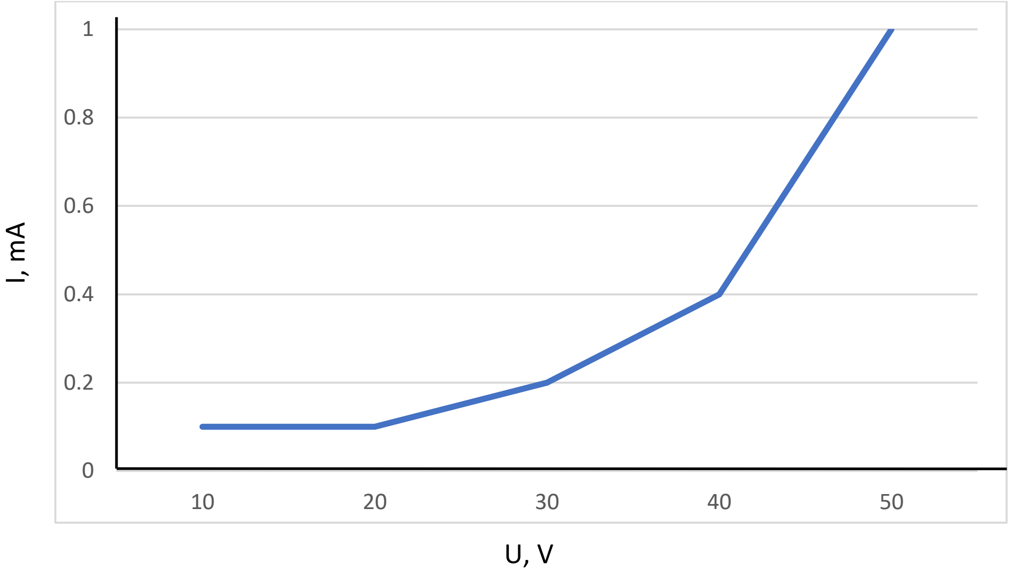

Figure 1. Current-voltage characterıstic of iodine-doped PMMA.

Determination of slopes and conductivity modes. The analysis of slopes $lgI - lgV$allows us to identify three characteristic modes: Ohmic mode $(n \approx 1)$– implemented at low voltages; Space-limited current mode (SCLC) $(n \approx 2)$– occurs at medium voltages; Trap -limited mode (TCLC) *(* $n > 2$, in this_case $n \approx 4$*)* – is realized at high voltages.

Transition from SCLC mode to TCLC corresponds to the trap filling voltageV_{TFL}.

DISCUSSION

The role of polyiodide complexes. When PMMA is doped with iodine, electrons are captured by molecular iodine, forming anionic forms. I^-.In the presence of excess, I_2 more complex polyiodide complexes are formed I_3^- и I_5^-.. These complexes are not part of the covalent structure of the polymer, but are localized in the interchain regions and near the polar groups of PMMA, creating trap energy levels in the band gap.

Shallow traps associated with I^-determine the initial conductivity and ohmic mode. Medium-depth traps associated with stable triiodide ions I_3^-, lead to the formation of the SCLC mode . With a further increase in voltage, deep traps associated with are activated, causing a transition to the I_5^-,TCLC mode and a sharp increase in the nonlinearity of the I-V characteristic.

Comparison with silicon. In crystalline silicon, charge transfer occurs via band carriers (electrons and holes), and doping creates donor and acceptor levels near the band edges. In iodine-doped PMMA, the situation is fundamentally different: charge transfer is injection -trap in nature and is determined by the filling and emptying of localized states of polyiodide origin. Therefore, it is advisable to analyze the I–V characteristics of PMMA using the SCLC and TCLC models rather than the band model .

Possible contribution of the Poole-Frenkel effect. At high voltages, the field emission of carriers from traps (the Poole-Frenkel effect) can additionally contribute to the current. However, the presence of clear linear sections with integer slopes in the graph $lgI - lgV$indicates the dominance of trap-limited mechanisms (SCLC / TCLC), and the PF effect should be considered an additional factor enhancing the current in high fields.

CONCLUSIONS

1. In iodine-doped PMMA, a multi-stage current flow mechanism is realized, including ohmic mode, SCLC and TCLC .
2. Slope analysis $lgI - lgV$allows for the reliable identification of these modes.
3. SCLC regime is associated with the dominance of intermediate-depth traps associated with ionsI_3^-.
4. TCLC mode is due to the contribution of deep traps characteristic of polyiodide complexesI_5^-.
5. The conduction mechanisms in iodine-doped PMMA are fundamentally different from the band mechanisms in silicon and should be analyzed within the framework of the injection - trap model.

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