EPR MEASUREMENTS OF POLYACETYLENE PREPARED IN THE MAGNETIC FIELD

ЭПР ИЗМЕРЕНИЯ ПОЛИАЦЕТИЛЕНА, ПРИГОТОВЛЕННОГО В МАГНИТНОМ ПОЛЕ

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The comparison of the EPR spectra of undoped polyacetylene prepared by the classical method and the EPR spectra of the oriented undoped polyacetylene prepared in the magnetic field is given.

The various properties of non-oriented polyacetylene have been extensively studied for a few years because of their importance for the understanding of this conjugated polymer [1—3]. The polyacetylene $(CH)_x$ is in the first approximation the one dimensional organic matter.

Recently, new methods have been used during the process of polymerization with the aim to produce the highly oriented polyacetylene [4—7]. In such a prepared doped polyacetylene the large parallel conductivities are reported e.g. by [5, 8]. One of the methods of gaining the oriented polyacetylene is the polymerization under the high magnetic field. This paper gives only a small contribution to the EPR investigation of polyacetylene prepared by the mentioned method.

The classical samples of undoped polyacetylene were prepared according to the technique of Shirakawa et al. [9]. The second group of samples was prepared in the external magnetic field for the purpose of the alignment of fibrils. The value of the magnetic induction was $B_{ext} = 0.3$ T. The so prepared samples were kept in a nitrogen atmosphere. Powdered samples as well as polyacetylene films were used in the EPR measurements.

The EPR spectra of both groups of polyacetylene samples were measured by means of the Bruker 200E-SRC spectrometer with a 100 kHz modulation in the X-band. For the angular dependences the EPR spectrometer with the goniometer was used.

The EPR spectra of all the investigated samples at room temperature were recorded. The EPR spectra formed simple symmetrical lines. The lineshape of all the measured spectra was of the Lorentzian type. The lineshapes were determined by a direct comparison of the experimental spectra with theoretical lines.

The calculated value of g-factor, obtained from Eq.:

$$g = \frac{hf}{\beta B_0} \tag{1}$$

(where h — is Planck's constant, f — the frequency of the microwave field, β — the Bohr magneton,

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Table 1

Samples No	The amplitude of the absorption derivative line I'_0 (rel. unit)	The linewidth ΔB_{max} [mT]	The relative concentrations of the paramagnetic centres $I'_0 \cdot \Delta B^2_{max}$
1	0.90	0.68	0.42
2	0.38	0.77	0.22

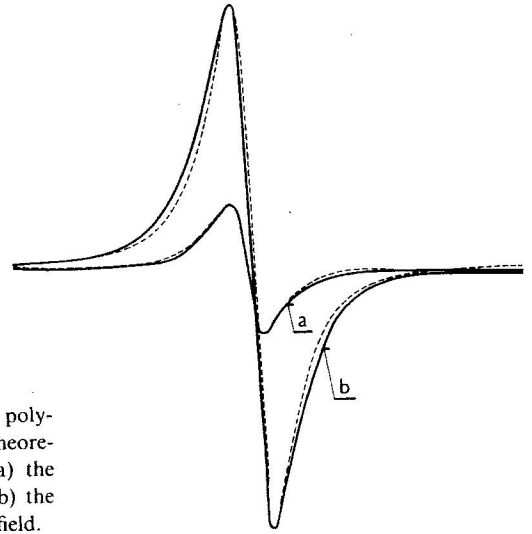

Fig. 1. Experimental EPR spectrum of polyacetylene (solid lines) compared with the theoretical Lorentzian curve (broken lines): a) the sample prepared in the magnetic field; b) the sample prepared without the magnetic field.

B_0 — the magnetic induction coordinated to the maximum of an absorption line) was $g = 2.0027$, and did not change in the comparable samples.

The values of the linewidth ΔB_{max}, defined as a peak-peak distance of an absorption derivative line, are given in Table 1.

The relative concentrations of the paramagnetic centres were evaluated as the products of $I'_0 \cdot \Delta B^2_{max}$, where I'_0 is the amplitude of the absorption derivative line. These values are also given in Table 1.

The results of our measurements can be summarized as follows:

The linewidth of the samples No 2 (prepared in the magnetic field) is greater (about 0.1 mT) than the value of ΔB_{max} for the samples No 1 (prepared without the magnetic field). This means that the spin mobility in the samples prepared in the magnetic field decreased.

The number of spins in the samples prepared in the magnetic field decreased enough compared with the spin number of the classical samples of polyacetylen. The relative change of the number of the paramagnetic centres is $N_1/N_2 \doteq 1.85$.

The angular properties of the EPR spectra of the transpolyacetylene film prepared in the external magnetic field (with the mark of the direction of the external magnetic induction) were performed too. The EPR spectra during the rotation of the sample in the EPR spectrometer (equiped with the

goniometer) were recorded. No anisotropy of EPR spectra was found the spectra recorded at various angles were the same. Probably, the value of the external magnetic induction was relatively small for the orientation effect of the magnetic field to appear on the spin orderlines.

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