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Optical, Transport and Magnetic Properties of Durham Polyacetylene

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OPTICAL, TRANSPORT AND MAGNETIC PROPERTIES OF
DURHAM POLYACETYLENE

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Abstract We present the results of optical transmission, AC and DC conductivity and ESR experiments on films of Durham route polyacetylene. While the properties of doped films resemble those of Shirakawa polyacetylene, those of the undoped polymer show differences which may be related to the short conjugation length of the Durham material.

INTRODUCTION

Transformation of the precursor BTFM-TCDT¹ gives dense films of polyacetylene without catalyst residue. Resonant Raman spectroscopy shows a predominance of short conjugated chains² comprising 30 - 40 (CH) units, so that it is unlikely that solitons are the dominant defect species. Doping reactions are relatively slow because of the dense morphology of this material³.

OPTICAL AND INFRA-RED PROPERTIES

The optical gap in fully isomerised Durham polyacetylene is higher than that observed in the Shirakawa polymer, and the absorption peak lies at 2.3 eV rather than 1.8 - 2.0 eV, in agreement with Raman data showing short conjugation lengths. Doping induces mid-gap features (figure 1), but at 1 eV rather than 0.75 eV. The infra-red dopant induced features are similar to those found in Shirakawa polyacetylene⁴, showing a broad band at 900 cm⁻¹, and a

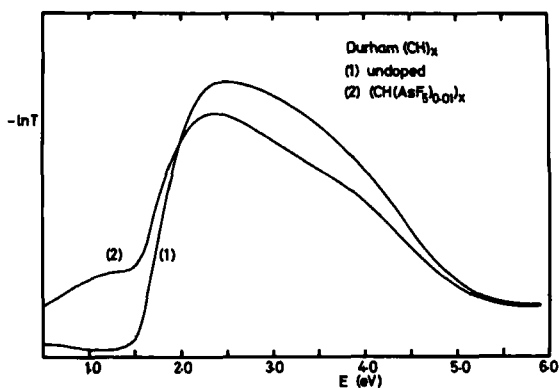


FIGURE 1 Optical transmission of undoped and AsF_5 doped Durham polyacetylene.

narrow band at 1370 cm^{-1} .

CONDUCTIVITY

The DC room temperature conductivity of Durham polyacetylene is $10^{-7}\text{ }(\Omega\text{cm})^{-1}$, an order of magnitude lower than that of Shirakawa poly-

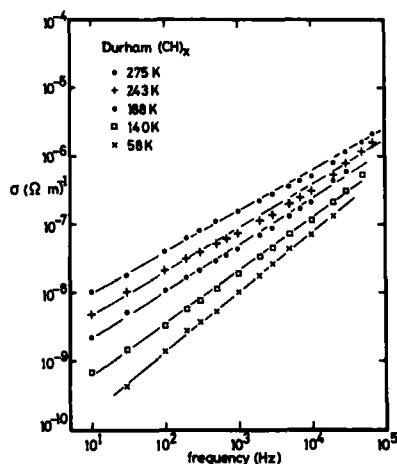


FIGURE 2 AC conductivity of Durham polyacetylene.

acetylene. The temperature dependence of conductivity can be fitted at low temperature to a relationship of the form $\sigma \propto \exp-(T_0/T)^{1/4}$, with $T_0 = 10^{10}$ K, compared with $2 \cdot 10^9$ in Shirakawa material. Above room temperature, conduction is activated with $E_a = 0.4$ eV. The low temperature AC conductivity, shown in figure 2, displays $\sigma \propto \omega^S$ behaviour with an exponent of about 0.8 between 10 Hz and 100 kHz, but the temperature dependence is activated ($E_a = 0.15$ eV), rather than the T^n dependence observed by Epstein et al.⁵

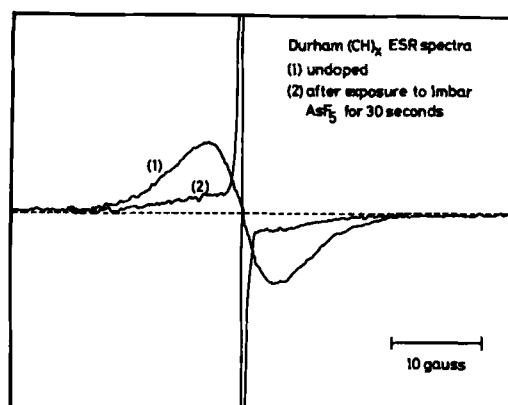


FIGURE 3 ESR signal of the Durham polymer before doping and after 0.1% AsF₅ doping.

ESR

Undoped films of trans-polyacetylene show a broad line at $g=2.0010$ with an intensity corresponding to about one spin per 2000 (CH) units. The line reaches its final magnitude after a few hours of the transformation reaction, and broadens only slightly between room temperature and 4K. Very light AsF₅ doping removes the broad line, and produces a narrow (0.3G) line (figure 3), with χ reduced to 1% of its original value. Iodine vapour doping reduces the line

intensity as doping proceeds, but there is no change in the width or profile of the line.

CONCLUSIONS

The properties of doped Durham polyacetylene strongly resemble those observed in the Shirakawa polymer. Those of the undoped polymer are related to the predominance of short conjugated sequences in the material.

This work will be presented in greater detail elsewhere.

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