Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

New Transport Mechanisms for Conducting Polymers: The Role of Disorder

Philip Phillips [a] & H.-L. Wu [a]

[a] Department of Chemistry, Massachusetts Institute of Technology, Rm. 6-223, Cambridge, Mass, 02139

Version of record first published: 04 Oct 2006.

To cite this article: Philip Phillips & H.-L. Wu (1992): New Transport Mechanisms for Conducting Polymers: The Role of Disorder, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 218:1, 261-261

To link to this article: http://dx.doi.org/10.1080/10587259208047050

Mol. Cryst. Liq. Cryst. 1992, Vol. 218, p. 261
Reprints available directly from the publisher
Photocopying permitted by license only

Printed in the United States of America

New Transport Mechanisms for Conducting Polymers: The Role of Disorder

Philip Phillips and H.-L. Wu
Department of Chemistry, Rm. 6-223, Massachusetts Institute of Technology, Cambridge, Mass. 02139

Abstract: A unified view of the metallic state in polyaniline and heavily-doped polacetylene is presented. We first consider a single randomly-protonated strand of the emeraldine form of polyaniline. We show explicitly that the disorder inherent in this system is described by the random-dimer model of Dunlap, Wu and Phillips[1]. The random dimer model is simply a tight-binding model for a binary alloy in which pairs of lattice sites are assigned one of two values at random. The random dimer model is shown to possess a narrow band of conducting states that can ultimately lead to dramatic increases in the conductivity if the Fermi level is appropriately tuned. It is demonstrated explicitly that the location in the energy band of the conducting states of the random-dimer model for polyaniline coincides with recent calculations of the location of the Fermi level in the protonated form of the polymer[2,3]. We argue then that the random-dimer model is capable of explaining the insulator-metal transition in polyaniline. In the context of polyacetylene, we propose a 'dirty metal' picture for the metallic state which is consistent with both the closing of the band gap and the existence of a band of extended states. Our model is based on the observation that a random distribution of solitons closes the band gap at ~5-6% doping and is formally equivalent to the random dimer model. The location of the extended states in the disordered soliton lattice is computed. It is shown that because these states lie in the vicinity of the band edge, they are capable of explaining the sudden onset of the experimentally-observed Pauli susceptibility and the subsequent depinning of the solitons in the metallic state. We close by noting that because the random dimer model applies to any lattice in which the defects are extended and possess a plane of symmetry, it quite generally describes any polymeric system in which the stable defects are solitonic or bi-polaronic in nature.

[1]D. H. Dunlap, H. L. Wu, and P. Phillips, Phys. Rev. Lett. 65, 88 (1990).
[2]H.-L. Wu and P. Phillips, Phys. Rev. Lett. **66,** 1366 (1991).
[3]P. Phillips and H.-L. Wu, Science **252**, 1805 (1991).