A time-domain analysis of dipolar effects in copper phthalocyanine thin films on indium–tin–oxide substrates

I Thurzo et al 2004 Semicond. Sci. Technol. 19 1075-1080 doi:10.1088/0268-1242/19/9/001

I Thurzo, G Pham and D R T Zahn

Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany E-mail: <u>ilja.thurzo@physik.tu-chemnitz.de</u>

Abstract. Transient charging in response to pulsed bias of copper phthalocyanine (CuPc) organic thin films on indium-tin-oxide (ITO) was investigated by charge transient spectroscopy (OTS) in situ under ultra-high vacuum conditions. The charge relaxation phenomena in response to a bias pulse are modelled in terms of dipolar effects, considering alternatively possible orientation of the dipoles (polarization) under an applied external electric field and capture of charge carriers in dipole-induced electron states. Assuming a Gaussian energetic distribution of the density of states (DOS) as a consequence of disorder, a simple formalism is derived to determine the width (variance) σ_d of the DOS from QTS data. The isothermal QTS response of single-layer Ag/CuPc/ITO samples provides evidence for dipolar effects in CuPc, an example of using the new formalism in practice. The dipole moment of the CuPc molecule proved to be too small for the assignment of the amount of transient charges to the reorientation of dipoles. The model of trapping of charge carriers at a Gaussian DOS induced by polar molecules in a non-polar solid has mediated an estimate of the fraction of polar molecules from the experimentally assessed variance σ_d of the Gaussian DOS. The resulting dependence of σ_d on the dipole moment is in striking coincidence with literature data related to other types of polar molecules in molecular glasses.

Print publication: Issue 9 (September 2004) Received 15 April 2004 Published 28 July 2004

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