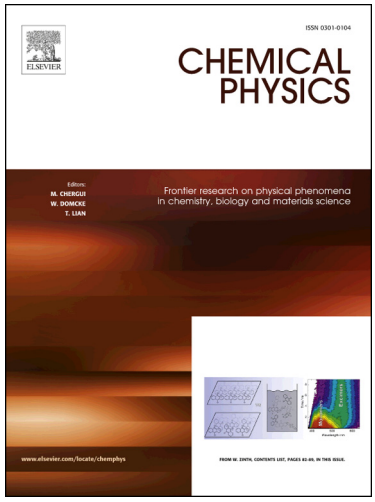

Effect of molecular optical vibrations on thermoluminescence of silicon organic polymer

V.I. Sugakov, N.I. Ostapenko

PII: S0301-0104(15)00124-X
DOI: http://dx.doi.org/10.1016/j.chemphys.2015.05.001
Reference: CHEMPH 9306

To appear in: *Chemical Physics*

Received Date: 24 November 2014
Accepted Date: 3 May 2015

Please cite this article as: V.I. Sugakov, N.I. Ostapenko, Effect of molecular optical vibrations on thermoluminescence of silicon organic polymer, *Chemical Physics* (2015), doi: http://dx.doi.org/10.1016/j.chemphys.2015.05.001

Effect of molecular optical vibrations on thermoluminescence of silicon organic polymer

V.I. Sugakov[a*], N.I. Ostapenko[b]

[a] Institute for Nuclear Research, National Academy of Science of Ukraine, 47 Nauki pr., 03680 Kyiv, Ukraine

[b]Institute of Physics, National Academy of Science of Ukraine, 46 Nauki pr., 03028 Kyiv, Ukraine

The paper proposes a model explaining the recently observed in [Chem. Phys. 394 (2012) 36] coincidence of the activation energies of charge carrier traps in thermoluminescence of a pure polymer poly(di-n-hexylsilane) with the energies of the vibrational modes seen in Raman spectra. The model is based on the fact that the thermal equilibration occurs after illumination much faster in the vibrational subsystem as compared to the electron level subsystem. Transitions between the trapped charge carrier states accompanied by the disappearance of an optical vibration quantum are investigated. It is shown that localized charge carrier, depth of which coincides with the energy of the optical vibrational quanta, may escape the traps due to these transitions and give the contribution to thermoluminescence. The suggested model explains the observed discrete character of the activation energies in the system with the quasi-continuous spectrum of traps and predicts the appearance of a structure in TSL curve.

Keywords: polymer, thermoluminescence, poly(di-n-hexylsilane), molecular vibration, activation energy

1. Introduction

The study of the fractional low temperature thermostimulated luminescence (TSL) provides important information about the presence and the nature of traps and defects for charge carriers in silicon organic polymers that are promising materials for the transport [1] and luminescent layers in electro-optical devices [2]. One of the processes determining the properties of TSL is the process of the charge carriers' escape from traps. In order to leave a trap and transit to a state with the energy above the mobility threshold a charge carrier has to acquire some additional energy. Moving, subsequently, it has a chance to encounter a localized charge of the opposite sign. The following recombination contributes to the TSL. Various mechanisms of the escape exist depending on the system and the type of the trap. Studies of polymers in a number of papers have revealed a connection between TSL processes and the processes of molecular relaxation: motion of the molecular groups connected to the polymer backbone, and other similar processes [3-10]. Manifestations of the molecular vibrations in the TSL are close to the features of other phenomena: thermostimulated currents, thermostimulated depolarization, glass transitions and melting as well as processes of the molecular relaxation. In some cases positioning of the TSL temperature peaks does not depend on the type of the impurities and is rather determined by the polymer matrix [7]. The molecular vibrations manifest themselves in various optical properties of polymers: in absorption, luminescence, Raman scattering. Yet, until recently the connection between optical phenomena and TSL features has not been observed.

---

* Corresponding author. Tel.: +380 (44) 5254810; fax: +380 (44) 5254463.
E-mail address: sugakov@kinr.kiev.ua (V.I. Sugakov)