Weierstraß-Institut
für Angewandte Analysis und Stochastik
Leibniz-Institut im Forschungsverbund Berlin e. V.

Preprint ISSN 0946 – 8633

Self-heating, bistability, and thermal switching in organic semiconductors

Axel Fischer[1], Paul Pahner[1], Björn Lüssem[1], Karl Leo[1], Reinhard Scholz[1],

Thomas Koprucki[2], Klaus Gärtner[2], Annegret Glitzky[2]

submitted: September 19, 2012

[1] Institut für Angewandte Photophysik (IAPP)
Technische Universität Dresden
George-Bähr-Straße 1
01069 Dresden, Germany
E-Mail: axel.fischer@iapp.de
paul.pahner@iapp.de
bjoern.luessem@iapp.de
karl.leo@iapp.de
reinhard.scholz@iapp.de

[2] Weierstraß-Institut
Mohrenstraße 39
10117 Berlin
Germany
E-Mail: thomas.koprucki@wias-berlin.de
klaus.gaertner@wias-berlin.de
annegret.glitzky@wias-berlin.de

No. 1735
Berlin 2012

2010 *Mathematics Subject Classification.* 82D37, 80A20, 34C55.

2008 *Physics and Astronomy Classification Scheme.* 81.05.Fb, 73.61.Wp, 72.80.Le.

Key words and phrases. Organic semiconductor, C_{60}, Joule self-heating, S-shaped negative differential resistance (SNDR), thermal switching, bistability, hysteresis, Arrhenius-like conductivity law.

The work leading to these results has been received founding from the Deutsche Forschungsgemeinschaft (DFG) within the collaborative research center SFB 787 Semiconductor Nanophotonics (Th. Koprucki), DFG Research Center MATHEON under project D22 (A. Glitzky), and by the European Communitys Seventh Framework Programme under Grant Agreement No. FP7-267995 — NUDEV— (A. Fischer).

Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 20372-303
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract. We demonstrate electric bistability induced by the positive feedback of self-heating onto the thermally activated conductivity in a two-terminal device based on the organic semiconductor C_{60}. The central undoped layer with a thickness of 200 nm is embedded between thinner n-doped layers adjacent to the contacts minimizing injection barriers. The observed current-voltage characteristics follow the general theory for thermistors described by an Arrhenius-like conductivity law. Our findings including hysteresis phenomena are of general relevance for the entire material class since most organic semiconductors can be described by a thermally activated conductivity.

Temperature-activated processes are omnipresent, e.g. in chemical and biochemical reactions or charge carrier and exciton transport and trapping dynamics in solids. Current flow through a solid generates Joule heat, resulting in an increased temperature with respect to the environment. In materials with a positive temperature coefficient of the conductivity, a rising temperature induces a current enhancement and an increased power dissipation, so that this electrothermal feedback loop favors a self-heating mechanism limited by heat losses towards the surroundings. This self-heating phenomenon was first studied in the investigation of the electrical breakdown of dielectrics induced by a thermal runaway [1, 2], where above a certain threshold voltage the cooling of the device is no more sufficient to keep the system in a stationary state. Furthermore, self-heating induces many thermal runaway and switching phenomena, including chemical reactions [3], thermistors [4, 5], semiconductors [6, 7], and transport through thin films [8, 9, 10]. Here, we show that thermal runaway phenomena are also crucial for the materials class of organic semiconductors, which is currently intensively investigated due to its interesting physics and promising device applications.

For materials with Arrhenius-like conductivity laws, self-heating phenomena only occur for activation energies $E_a > 4\,k_\mathrm{B}T_a$, where k_B denotes Boltzmann's constant and T_a the ambient temperature, see [11]. A characteristic feature of organic semiconductors is a temperature activated conductivity arising from hopping transport. Typically, the mobility μ of carriers follows a law $\mu \propto \exp(-\mathrm{const}/T^n)$, where n varies between 1 and 2 depending on the charge carrier concentration [12]. In disordered organic semiconductors, the density of states can be described by a Gaussian proportional to $\exp[-\frac{1}{2}(E-E_0)^2/\sigma^2]$. The width σ is usually in the range between $2\,k_\mathrm{B}T_a$ and $6\,k_\mathrm{B}T_a$, resulting in activation energies of $4\,k_\mathrm{B}T_a$ to $36\,k_\mathrm{B}T_a$ [13]. At interfaces between the organic materials and metallic contacts, injection barriers up to several tenths of an eV result either in thermionic injection or in the formation of a Schottky barrier. It is common practice to reduce these injection barriers by doping the layers adjacent to the contacts, resulting in Arrhenius-like conductivity-temperature laws [14].

Surprisingly, even though activation energies above $4\,k_\mathrm{B}T_a$ are quite common in organic semiconductors, the positive feedback between Joule heating and a subsequent thermal runaway has not been observed yet. The crucial role of Joule heating on the device performance has already been considered for fast rectifying diodes [15] and for organic light-emitting diodes (OLEDs) [16]. However, in these devices a thermal runaway was probably inhibited by a series resistance within the circuit, arising e.g. from an indium-tin-oxide electrode.

Here, we demonstrate electrothermal bistability for vertical crossbar structures based on the organic semiconductor C_{60}. It is shown that an abrupt turnover from a low conductive to a highly conductive state follows in a natural way from the current-voltage characteristics predicted by theory.

First, we summarize the theory of self-heating for a thermally activated conductivity and suppose in the following that the isothermal current-voltage relation for the circuit is given by a power law

$$I_{\mathrm{iso}}(U,T) = I_{\mathrm{ref}} \left(\frac{U}{U_{\mathrm{ref}}}\right)^{\alpha} F(T) \tag{1}$$

with a positive exponent α and a temperature-dependent conductivity factor $F(T)$ resulting from an Arrhenius law

$$F(T) = \exp\left[-\frac{E_a}{k_{\mathrm{B}}}\left(\frac{1}{T}-\frac{1}{T_a}\right)\right]. \tag{2}$$

The quantities U_{ref}, I_{ref}, and $P_{\mathrm{ref}} = U_{\mathrm{ref}} I_{\mathrm{ref}}$ denote reference values for voltage, current and power, respectively. The homogeneous steady states of the device are given by equilibria of the global heat balance equation expressing that the dissipated Joule power $\dot{Q}_2 = IU$ equals the heat loss $\dot{Q}_1 = \frac{1}{\Theta_{\mathrm{th}}}(T-T_a)$ to the surrounding described by the thermal resistance Θ_{th},

$$\frac{1}{\Theta_{\mathrm{th}}}(T-T_a) = P_{\mathrm{ref}} \left(\frac{U}{U_{\mathrm{ref}}}\right)^{\alpha+1} F(T). \tag{3}$$

The self-consistent current-voltage characteristic including self-heating parametrized by the temperature $T \geq T_a$ is obtained by combining Eqs. (1) and (3),

$$U(T) = U_{\mathrm{ref}} \left(\frac{T-T_a}{\Theta_{\mathrm{th}} P_{\mathrm{ref}}}\right)^{\frac{1}{\alpha+1}} F(T)^{-\frac{1}{\alpha+1}}, \tag{4}$$

$$I(T) = I_{\mathrm{ref}} \left(\frac{T-T_a}{\Theta_{\mathrm{th}} P_{\mathrm{ref}}}\right)^{\frac{\alpha}{\alpha+1}} F(T)^{\frac{1}{\alpha+1}}. \tag{5}$$

Different points on the self-consistent current-voltage characteristic correspond to different values of the temperature rise $T - T_a$. The differential resistance of this S-shaped curve has the form

$$\frac{dU}{dI} = \frac{1-(T-T_a)\frac{d}{dT}\ln F(T)}{\alpha+(T-T_a)\frac{d}{dT}\ln F(T)}\,\frac{U}{I}. \tag{6}$$

For $T - (\frac{d}{dT}\ln F(T))^{-1} > T_a$ a region of negative differential resistance (NDR) is obtained. In the Arrhenius type temperature dependence Eq. (2) a NDR region only appears for activation energies $E_a > 4\,k_{\mathrm{B}}T_a$. This can be seen in Fig. 1 where the self-consistent IV curve of such an intrinsic device is shown for an isothermal Ohmic current-voltage relation ($\alpha = 1$, $U_{\mathrm{ref}}/I_{\mathrm{ref}} = 2000\,\Omega$) The turnover points of the S-shaped IV curve are characterized by the condition $\frac{dU}{dI} = 0$. For $E_a > 4\,k_{\mathrm{B}}T_a$, irrespective of the exponent α in Eq. (1), the temperature increase $\Delta T_{1,2} = T_{1,2} - T_a$ at the two turnover points becomes

$$\frac{\Delta T_{1,2}}{T_a} = \frac{E_a}{2k_{\mathrm{B}}T_a}\left(1 \mp \sqrt{1-\frac{4k_{\mathrm{B}}T_a}{E_a}}\right) - 1. \tag{7}$$

The temperature rises at the turnover points depend only on the normalized activation energy, $E_a/(k_{\mathrm{B}}T_a)$. Along the S-shaped current-voltage characteristics, two stable branches exist: a highly conducting 'ON' state and a low conducting 'OFF' state, whereas the intermediate NDR region is unstable, see Fig. 1. This bistable behavior of the IV characteristic is related to thermal switching at the turnover points with $dI/dU \to \infty$, involving a hysteresis loop [17, Ch. 6.2], where