A Model for Charge Transport in Amorphous GST Based on a Modified Variable-Range Hopping Process

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ABSTRACT

Starting from experimental results and first-principle simulations we have developed a transport model for amorphous chalcogenides based upon a hopping process among traps. The conduction mechanism is suitably modeled by means of a generalization of the variable-range hopping, and studied stochastically through Monte Carlo simulations. The transition rates available in the literature have been modified by incorporating the effects of the local electric field. The improved model is able to reproduce the S-shaped current-voltage characteristics of these materials.
Simulations have shown that the snap-back effect in the $J(V)$ curve can be ascribed to the formation of domains of opposite charges within the material close to the contact region, acting as a positive feedback for carriers. A microscopic particle description is also used to detect the formation of filaments inside the chalcogenide material.

Key words: amorphous chalcogenides, charge-transport model, current-driven Monte Carlo simulation, phase-change memories.

1. INTRODUCTION

The need for new, compact, high-density, reliable storage devices represents a challenge for modern electronics. Non-silicon materials like GST chalcogenides have been investigated for decades. Nowadays they represent the standard technology for optical storage due to the easiness to obtain the phase transition that makes them to switch between the ON/OFF states. More recently an intense effort has been carried out to use such materials also in the solid-state memory technology.
By means of experimental structural data[1,2] and first-principle studies[3-6] it was found that the long-range disordered atomic structure of amorphous chalcogenides implies the presence of a large concentration of localized states. On the microscopic scale the localized states originate from structural defects like dangling bonds and vacancies, and may give rise to either donor- or acceptor-like traps. From these considerations one may assume that an appropriate model for electric conduction in chalcogenide glasses must consider a trap-controlled transport process,[7-9] namely, a hopping of charge carriers through localized states.
In the following sections we present a model based on a modified variable-range hopping process, an early version of which was presented at E*PCOS 2008. A more detailed and comprehensive discussion of the results, including considerations about the conditions for threshold switching and the formation of filaments, is also given.

2. THE PHYSICAL MODEL AND THE SIMULATIVE FRAMEWORK

The model is based on the assumption that a carrier can hop among traps in the chalcogenide region through direct or thermally-assisted tunneling.[10,11] Within such a conduction framework, a 3D model of charge transport due to electron hopping among donor-type traps has been implemented using a Monte Carlo procedure. As test case we

consider a simple device made of a layer of amorphous GST in contact with two metallic electrodes, as sketched in Fig. 1.

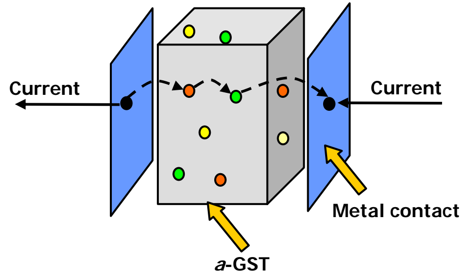


Figure 1 – Sketch of the modeled device: an *a*-GST region of length ℓ is sandwiched between two metallic planar electrodes of cross sectional area Σ.

Due to the amorphous nature of the material under investigation, traps have randomly been positioned inside the sample, and an energy level E_i, chosen at random within a narrow band of width ΔE is ascribed to each trap. Traps can host only one carrier at a time: they are positively-charged if they can still host an electron, otherwise they are neutral. A second set of negatively charged traps, corresponding to acceptor states that compensate the material, are also considered in order to guarantee the electrical neutrality. These traps are always filled by carriers and do not contribute to the transport process.

Contacts are represented by two infinite reservoirs of both carriers and empty states: they can at any time inject electrons into the traps or host electrons coming from them.

Transitions between traps, from traps to contacts and from contacts to traps are accounted for following the variable-range hopping theory.[9] The transition rate S_{ij} for an electron hopping from an occupied site *i* to an empty site *j* is evaluated according to the following equation:

$$S_{ij} = \begin{cases} \nu_0\, T_{ij} \exp\left(-\dfrac{\Delta\varepsilon}{k_B T}\right) & \text{if } \Delta\varepsilon > 0 \\ \nu_0\, T_{ij} & \text{if } \Delta\varepsilon \le 0 \end{cases} \qquad (1)$$

where ν_0 represents the attempt-to-escape frequency, T_{ij} is the transmission coefficient of the potential barrier between the sites *i* and *j*, which depends on the separation distance R_{ij} and on the height and shape of the barrier; $\Delta\varepsilon = E_j + e\varphi_j - E_i - e\varphi_i$ indicates the energy difference between the initial (E_i) and final (E_j) electron states, φ_i and φ_j being the electric potential associated to the *i*-th and *j*-th trap, respectively.

It should be pointed out that in the original formulation[12] of Eq. (1), the dependence of the energy barrier between the scattering centers on the electric field is missing. This is clearly not realistic for the case at hand. Here, T_{ij} is considered as proportional to the overlap integral of the exponential tails of the electron wave functions in the barrier region, this yielding:

$$\alpha^2 = \alpha_0^2 - \frac{m_0 \beta}{\hbar^2} \left|\varphi_i - \varphi_j\right| \qquad (2)$$

In Eq. (2) α_0 is the inverse of the characteristic tunneling distance at $\varphi = \text{const}$, m_0 the electron mass and β a phenomenological parameter, whose effect is discussed in section 3.

The standard voltage-driven Monte Carlo framework has been modified into a current-driven simulation necessary to investigate S-shaped characteristics. The implemented Monte Carlo procedure can be summarized as follows:

i) Traps are generated at random positions inside GST and are filled according to the equilibrium Fermi distribution; the charge on the planar contacts is initially zero. The simulation time t_s and the electron injection time t_I are set equal to zero.

ii) An electron is added to one contact. The time t_I is increased by $\Delta t_I = e/I$ (*e* and *I* being the electron charge and the prescribed current, respectively).

iii) The potential profile at any site and the voltage drop across the device are evaluated on the basis of the actual trap- and contact-occupancy configuration.

iv) The transition rate for any hopping process S_{ij} from site i to site j is evaluated by using the potential profile calculated at the previous step. The total hopping probability is evaluated as $S_{\mathrm{TOT}} = \sum_i S_i$, $S_i = \sum_j S_{ij}$.

v) A random number r is generated between [0,1] with uniform probability. The time of occurrence of the next hopping process is calculated as $\Delta t = -\ln r / S_{\mathrm{TOT}}$. The simulation time t_s is updated by Δt. If the updated simulation time t_s' exceeds the injection time t_I, the simulation time is set back to t_I and the procedure is cycled from step ii) without performing any further action; otherwise the new time $t_s = t_s'$ is accepted.

vi) The starting trap i is chosen according to the probabilities S_i and, subsequently, the arrival trap j is selected according to S_{ij}. Contacts are considered as additional traps.

vii) The carrier hopping from trap i to trap j is performed and the occupancy values are updated. If the total simulation time t_{MAX} is reached the numerical procedure is concluded, otherwise it is cycled from step iii).

The computation of the electric potential at the trap sites is of great importance in the model, due to the form of Eqs. (1) and (2). A fully 3D solution of the Poisson equation is necessary. A self-consistent solution of the Poisson equation brings about the non-negligible drawback of a very high computational load. The problem is tackled as follows. The local potential is calculated as the sum of two contributions: one accounting for donor and acceptor centers inside the *a*-GST, and one produced by the two contacts, the latter being always described as planes with a uniform charge density. When trap-to-trap transition rates are evaluated, the charged traps are modeled as 3D point-like Coulomb centers. When the trap(contact)-to-contact(trap) transition rates are calculated, the trap potential is modeled as that of a charge sheet placed at the trap position and parallel to the contact, with a total charge equal to the trap charge. Despite the approximation of the trap-electrode interaction to a 1D problem, the two main features of the computation, i.e., the correctness of the boundary conditions at the electrodes and the self-consistency between the electric potential and electron dynamics are preserved.

3. RESULTS & DISCUSSION

In Fig. 2 we report the $J(V)$ characteristic for the simulated device ($\ell = 27$ nm and $\Sigma = 900\,\mathrm{nm}^2$, see also the caption of Fig. 2) obtained by tuning the parameters of the model on experimental data[10]. For each simulation point a number of independent runs have been performed at a given current I and the results averaged.
Up to the threshold current, the shape of the $J(V)$ curve is in good quantitative agreement with the experimental one and it is also consistent with previously-developed analytical models.[10,13] The typical features of an *a*-GST current-voltage characteristic are reproduced by the model: an initial Ohmic region at the lowest currents, followed by a sub-threshold exponential region and, then, by a negative differential-resistance region where the potential difference between the contacts is reduced at increasing currents. The values of both voltage and current density at the snap-back point correspond to the experimental data.
At higher currents, the simulated curve shows a fast increase in the potential drop instead of a swift rise of the current, suggesting the existence of a limiting current. This behavior can also be theoretically predicted by a qualitative analysis of the equations, and is a consequence of a trap-limited transport scheme. A realistic transport model under these high-current conditions must account for other physical features like, e.g, band conduction.

The advantages of the Monte Carlo simulation can be fully exploited in the interpretation of the results, that can be analyzed in terms of a microscopic particle description (Figs. 3a and 3b). In the whole sub-threshold region, (corresponding to $J < 10^5\ \mathrm{A/cm^2}$), the occupation fraction is almost constant along the device around the value of 0.5, this meaning that the space charge due to donor and acceptor traps in the GST region is uniformly distributed and compensates on average. The charge on the contacts increases with J, thus creating a stronger electric field inside the device and allowing for long-range transitions, which become more and more probable due to the lowering of the energy barrier induced by the applied field. As the current increases, hopping process looses efficiency in transferring carriers from the GST region to the collecting contact, and charges tend to accumulate in the region close to the drain contact. As a consequence, an internal counter-field adds to the one generated by the two contacts, as shown in Fig. 3c. The initial linear drop existing between the two electrodes turns into a more complex shape resulting from the superposition of contributions coming from differently-charged regions. The net effect is the decrease in the electric field as the current increases, giving origin to the snap-back point. A higher

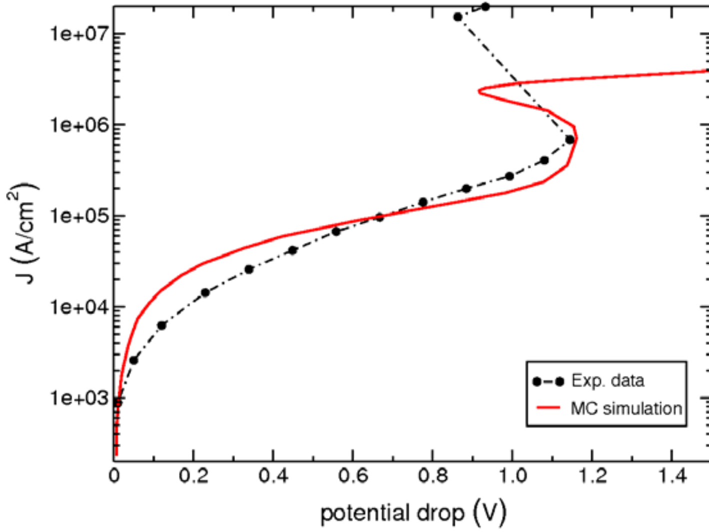


Figure 2 – Experimental and simulated $J(V)$ characteristics. The voltage values have been obtained as averages of the final output over 192 independent simulations per current step. The simulation time was adapted in each current step to ensure that the stationary potential profile is reached, varying it from 0.1 to 1 ns.
The parameters used for the Monte Carlo simulations are: $N_t = 1.48 \cdot 10^{19}\,\mathrm{cm}^{-3}, \nu_0 = 1.35 \cdot 10^{13}\,\mathrm{s}^{-1}, \alpha_0 = 4.54 \cdot 10^{6}\,\mathrm{cm}^{-1}$, and $\beta = 1/20$.

current can be sustained only with more frequent transitions. This is made possible by depleting the GST region close to the injection contact (the occupation fraction quickly goes down to values close to 0), and filling the region close to the collecting one (the occupation fraction rises up to values close to unity). As a consequence, the counter-field is enhanced and eventually produces the feed-back effect necessary for the snap-back of the current-voltage characteristic. When the occupation fractions have reached their limiting values, a further increase in the external current cannot be sustained any more, the charge accumulates indefinitely on the contacts and charge transport cannot take place any longer across the GST region at the desired rate.

As reported in the previous section, the model contains the following physical quantities and parameters: the trap concentration N_t, the attempt-to-escape frequency ν_0, the characteristic tunneling distance α_0, and the coefficient β. At present, most of them are unknown or known only qualitatively. From a complete analysis of the influence of each parameter on the $J(V)$ characteristics, we have found that only two of them play a key role in the occurrence of the snap-back effect: the trap concentration N_t and the β coefficient (see Figs 4a and 4b). They both influence the formation of domains of opposite charges in the two regions close to the electrodes. When the concentration of the traps is below $5 \cdot 10^{18}\,\mathrm{cm}^{-3}$, the switching behavior is not present: in this case the contribution from the two domains on the counter-field is not sufficient to originate the feed-back effect necessary for a negative differential-resistance behavior. When the number of traps inside the device increases above this value the snap-back effect becomes more and more evident. An even stronger influence on the shape of the $J(V)$ characteristic is provided by β, i.e., by the incorporation of the effects of the local electric field on the transition rates. By means of numerical simulations, also supported by analytical calculations, it can be demonstrated that if a constant value for α is considered (that is, by setting $\beta = 0$ in Eq. (2)), the current reaches an asymptotic value without a potential snap-back. This is understandable by considering that the local field plays the role of a lowering (or enhancing) agent for the energy barrier that confines a carrier in a trap site; in the framework of the modified variable-range hopping adopted here

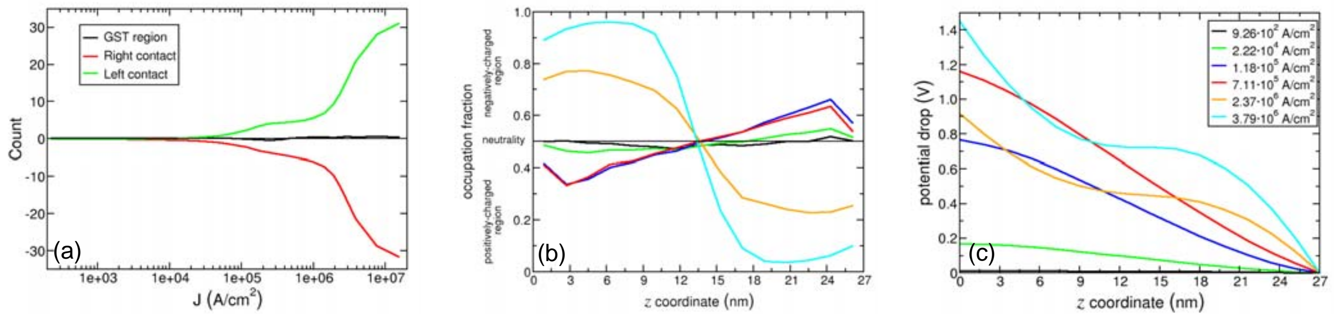


Figure 3 – Number of charges inside the device and on the two contacts (a); trap-occupancy fraction (b) and potential profile (c) along the longitudinal axis. For the two last plots, data have been collected averaging values over 15 1.8 nm-wide bins. Carriers enter the device from the right contact.

this means enhancing or decreasing the hopping probability through tunneling. When the α value calculated by means of Eq. (2) gets close to zero, long-range transitions become frequent and carriers are easily transferred across the device from one contact to the other. The transfer rate inside the device becomes higher than the one necessary to reach the collecting contact. Consequently, a negative domain facing the contact is formed, this contributing to the rise of the snap-back effect. As a rule of thumb given the value of α_0, the greater the value of β is chosen, the more evident the negative-differential resistance region is found. These considerations confirm the basic assumptions and the results found by a previous model.[10] The other parameters have a minor importance and may be used for a fine tuning of the simulated data.

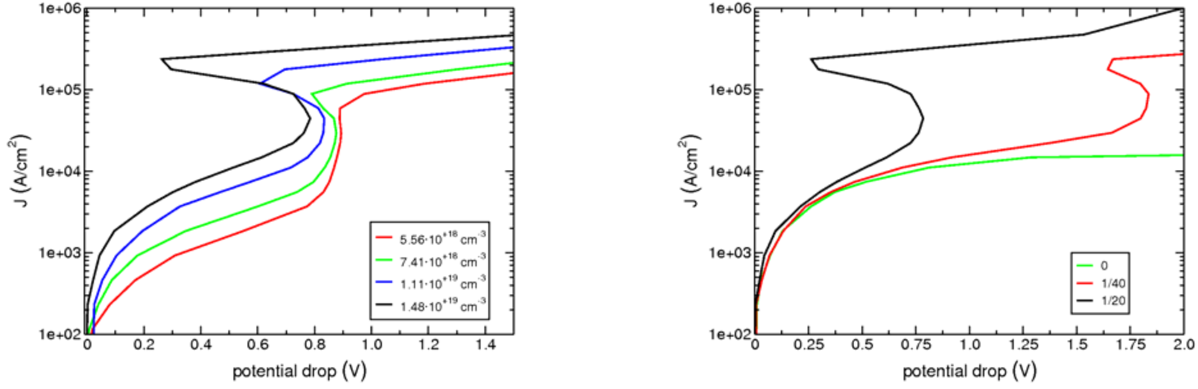


Figure 4 – Effect of the trap concentration N_t and of the β coefficient on the $J(V)$ characteristics. The other parameters are: $\nu_0 = 10^{12}\ \mathrm{s}^{-1}$, $\alpha_0 = 4.54 \cdot 10^6\,\mathrm{cm}^{-1}$.

It is often believed that S-shaped characteristics are generated by the formation of current filaments in the material, but a one-to-one correspondence between filamentation and S-shaped characteristics cannot *a-priori* be established. The latter can exists also without filaments.[14] The Monte Carlo investigation allows one to look at the trajectories followed by carriers while moving from one contact to the other one. In the four left panels of Fig. 5 we report the probability distribution of the number of hops needed to transfer from one side to the other one at increasing currents.

In the sub-threshold Ohmic region carriers pass through a high number of traps before reaching the collecting contact, moving often back-and-forth in a diffusive regime. The mean and the mode of the distribution are around 140 and 55 hops respectively, and the relative frequency never exceeds 0.65%. Things go differently as the current increases, as illustrated by the next panels. As soon as the snap-back condition is reached, a growing number of trajectories involve less and less traps, and many of them are concluded within 2 to 4 hops. The mean value of the hop distribution goes down to 8 for the last current points before the snap-back point and to 3 after it. A quasi-ballistic regime sets in: in all these cases the most frequent sequences involve only two intermediate traps. Further analyses have been performed in order to detect current filaments. Results are reported in the three right panels of Fig. 5. In the sub-threshold exponential region carriers usually fill traps close to the contacts, the first hop involving traps in the first half of the device and the second hop generally involving the second half. Such a behavior is a consequence of the effect of the internal electric field on the energy barriers between the traps and on the transition rates. Carriers are transferred from one contact to the other one by means of few long-range transitions and can tunnel across half the device (or more), thus enhancing the formation of opposite charge domains close to the contacts. After the snap-back point and the negative-differential resistance region, we have observed that traps in the mid of the device are more often visited than before, and also shorter transitions occur.

Going into more details, we have verified that the most frequent path is followed less than 3% of the times, which lets us conclude that under the tested conditions the transport process does not show evidences of preferred paths. On the contrary, we have found that a two- or three-step scheme involving a long-range transition and one or two short hops is often used.

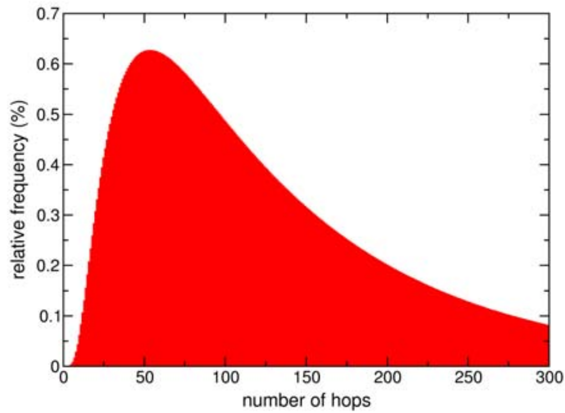
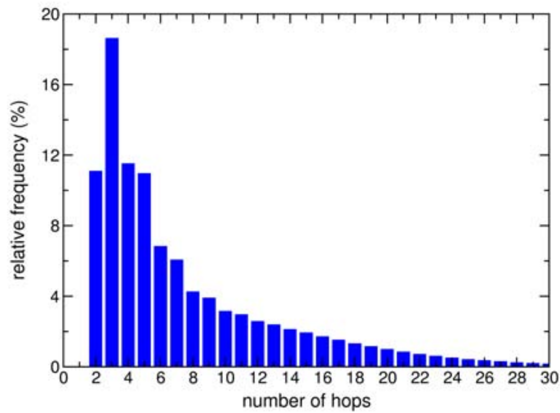
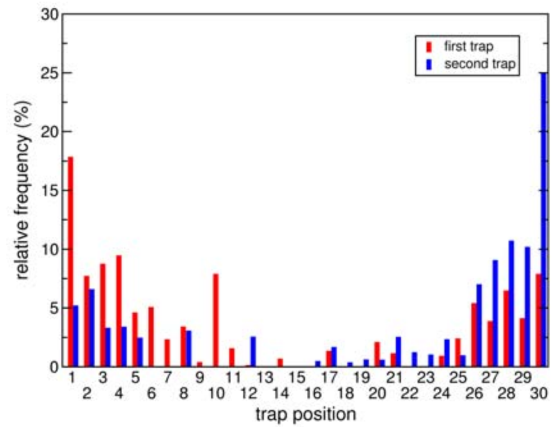
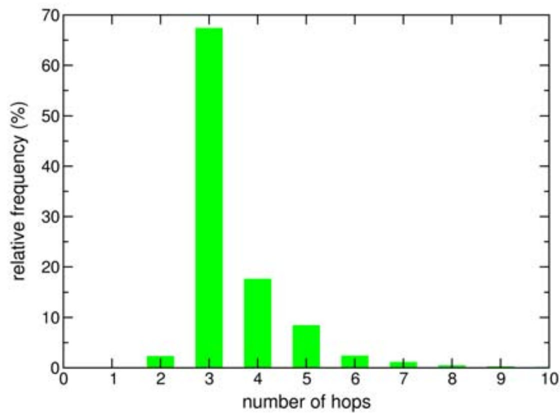


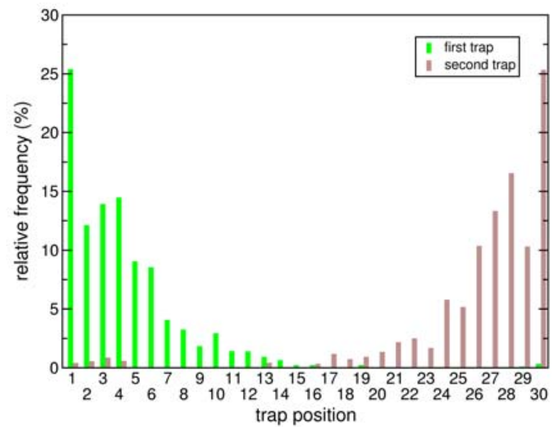
Figure 5 – Number of hops needed to transfer a carrier from one contact to the other (left) and position of the involved traps (right) for the most frequent case of three hops. Positions have been calculated by means of 30 bins into which the GST region has been subdivided. Carriers enter from the left.

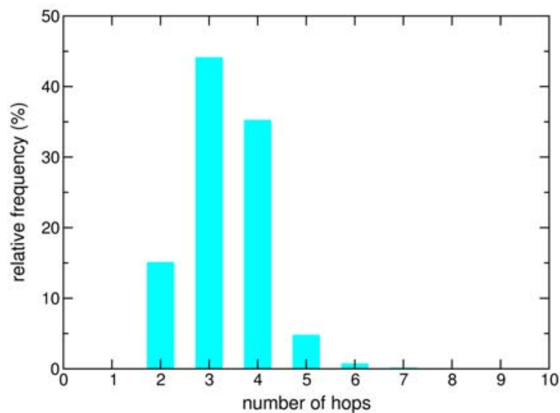
Moving from top to bottom, the distributions refer to the sub-threshold Ohmic regime (red), to the end of the exponential regime (blue), to the end of the negative-differential regime (green) and to the upper part of the *J*(*V*) characteristic (cyan), respectively.

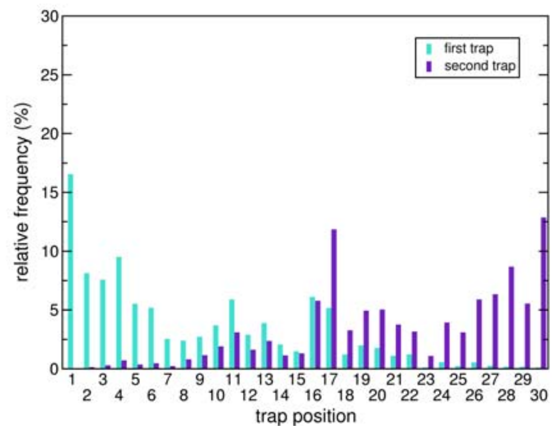












4. CONCLUSION

A trap-controlled conduction model for amorphous chalcogenides has been implemented through a Monte Carlo procedure, following the suggestion coming from experimental structural information and first-principle studies available in the literature. In our model carriers hop through a number of localized states featuring the material; transition rates are evaluated by means of a generalization of the Miller-Abrahams expression, obtained by adding a dependence of the transmission coefficient on the electric field. In order to correctly account for S-shaped characteristics, the standard voltage-driven Monte Carlo framework has been modified into a current-driven simulation. The results show that a realistic theoretical transport framework based on a modified variable-range hopping yields a complete microscopic description of the mechanism governing the threshold switching and an agreement with experimental data. Taking full advantage of the microscopic particle description of the Monte Carlo simulation it has been possible to interpret the switching effect by means of domains of opposite charge that originate close to the contacts. The possibility of current filaments have also been investigated.

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Biographyies

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Enrico Piccinini received the *Laurea cum laude* in Materials Engineering at the University of Modena and Reggio Emilia, Italy, in 2000, and the PhD in Chemical, Environmental Engineering and Safety at the University of Bologna, Italy, in 2004. Since 2004 he has been working with the Department of Electronics, Computer Science and Systems of the University of Bologna under a research contract. His research interests include the analysis of combined effects of dilation and mass transport in polymeric systems, numerical modelling of non-Fickian diffusion, the design and testing of prototype apparatuses for the simultaneous measurement of mass sorption, diffusion and dilation in polymeric films, theoretical and computational modelling of charge-transport properties in ion channels and newly-designed semiconductor materials by means of Molecular Dynamics and Monte Carlo simulation techniques.

Rossella Brunetti received the *Laurea cum laude* in Physics in 1981 and the PhD in Physics at the University of Modena, Italy, in 1987. She has been working at the Physics Department of the University of Modena and Reggio Emilia, Italy, as teaching and research assistant since 1990. From 2002 she is associate professor in Physics at the Physics Department and the Pharmacy Faculty of the same University. Past and present research interests include: theory of electron transport in semiconductors in semiclassical and quantum conditions, numerical-simulation techniques (mainly the Monte Carlo and Molecular Dynamics approaches) applied to the analysis of semiconductor structures and devices, quantum transport problems in mesoscopic structures and low-dimensional systems, and, more recently, ion conduction across nanometric ion channels of the cell membrane.

Massimo Rudan received the degree in electrical engineering in 1973 and the degree in physics in 1976, both from the University of Bologna, Italy. He joined the Department of Electronics (DEIS), University of Bologna, in 1975. In 1990, he was appointed Full Professor of Microelectronics. Since 1983, he has been working in a group involved in the investigations of the physics of carrier transport and numerical analysis of semiconductor devices. In 1985 to 1986 he was a Visiting Scientist at the IBM Thomas J. Watson Research Center, Yorktown Heights, NY, studying the discretization techniques for the higher-order moments of the Boltzmann transport equation. His research interests are in the physical and numerical modeling of nanodevices and of solid-state sensors. M. R. is Fellow of IEEE.

Carlo Jacoboni obtained his PhD in Physics in 1969 at Purdue University, West Lafayette, Indiana (USA). He is full Professor of Atomic Physics at the University of Modena and Reggio Emilia. He has published several books and about 160 scientific papers in international journals in the field of charge transport in semiconductors. He has been Director of several national and international Schools and Conferences on Transport in Semiconductors and Principal investigator of national and international Research Contracts. His scientific activity has been related to electron transport in semiconductor materials and devices and to the theory of quantum transport in mesoscopic structures in coherent and dissipative regimes. He is Fellow of the American Physical Society.