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To cite this article: E Piccinini *et al* 2009 *J. Phys.: Conf. Ser.* **193** 012022

View the article online for updates and enhancements.

Monte Carlo simulation of charge transport in amorphous chalcogenides

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Abstract. The $I(V)$ characteristics of amorphous GST devices show a peculiar S-shape behavior, that is a swift rise of the current along with a voltage snap-back. This type of characteristics led to a growing research interest in view of the future application of such materials to the manufacturing of phase-change memory devices. In this work we adopt a generalization of the variable-range hopping theory to simulate charge transport in a layer of amorphous $Ge_2Sb_2Te_5$ sandwiched between two planar metallic electrodes. The numerical implementation of a current-driven Monte Carlo code allows one both to provide a complete microscopic particle picture of electrical conduction in the device and to better analyze the mechanisms governing the snap-back effect.

1. Introduction

Chalcogenide materials are nowadays the focus of many research efforts owing to their application as phase-change materials in non-volatile memories. Particular attention has been devoted to the $Ge_2Sb_2Te_5$ (GST) compound that has been recognized as the most suitable for industrial applications. When the GST is in its amorphous phase, it exhibits a threshold switching in the conduction characteristic. The latter consists in a transition from a low- to a high-conductive state once the applied bias reaches a critical threshold voltage and an S-shaped negative differential resistance behavior in the I(V) curve is found [1]. The theoretical understanding of such a mechanism is crucial in view of the fabrication of innovative nonvolatile memories.

The transport properties of amorphous chalcogenides have been studied with different schemes relying either on a trap-controlled conduction [2, 3] or on the generation-recombination and impact ionization mechanisms via localized states [1]. The large concentration of localized states arising from structural defects and acting as donor- or acceptor-like traps has been shown by experimental and theoretical investigations [4, 5, 6]. This seems to indicate the essential role of trapped-carrier transitions in the electrical behavior of amorphous GST (a-GST).

2. Physical model and results

We have considered a device consisting of a 3D region of a-GST, with a cross section $\sigma = 270$ nm^2 and length $\ell = 27$ nm, sandwiched between two planar contacts, in which a number N_t of randomly-positioned donor-like traps exist. Carriers can hop among traps by tunneling. An energy-level, randomly chosen within a narrow band of widthΔ E centered at the Fermi level, is attributed to each trap. In order to mimic contacts, two infinite "reservoirs" of both carriers and empty states at the equilibrium Fermi energy have also been considered. The reservoirs can at any time inject electrons into the traps of the GST or host electrons coming from the GST. The electrical neutrality is ensured by fixed negative charges not involved in the transport process. The transition rate S_{ij} for a carrier's hopping from an occupied site i to an empty site j
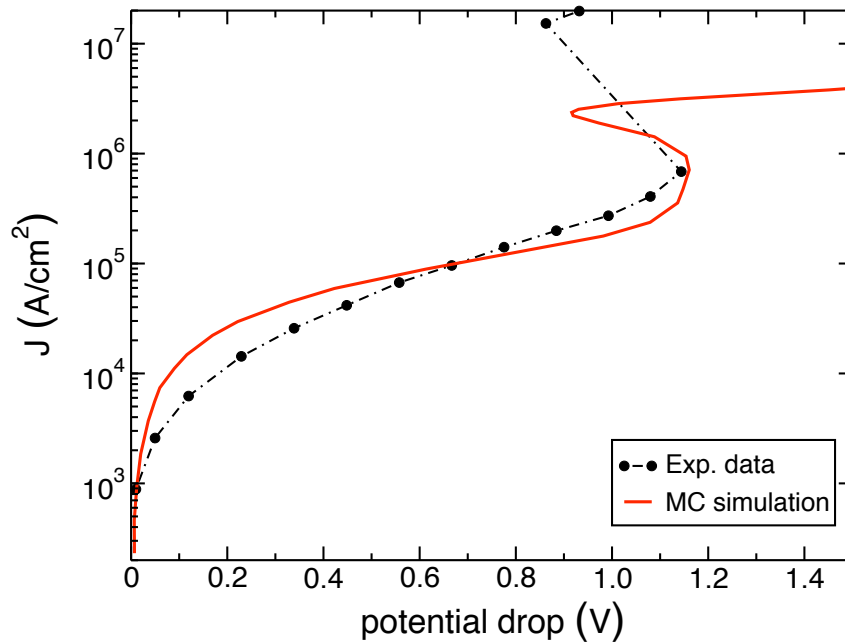

Figure 1. Measured and simulated current density vs voltage. The parameters used in the Monte Carlo simulations are: $\beta = 1/20$, $\nu_0 = 1.35 \cdot 10^{13}$ s^{-1}, $N_t = 1.48 \cdot 10^{19}$ cm^{-3}, and $\alpha_0 = 4.54 \cdot 10^6$ cm^{-1}. The experimental data are taken from Ref. [2]

is evaluated according to the variable-range hopping theory [7]:

$$S_{ij} = \begin{cases} \nu_0 \, T_{ij} \exp\left[-\dfrac{\Delta\epsilon}{k_B T}\right] & \text{if} \Delta \quad \epsilon > 0 \\[2mm] \nu_0 \, T_{ij} & \text{if} \Delta \quad \epsilon \leq 0 \end{cases}. \qquad (1)$$

Here, ν_0 is the attempt-to-escape frequency, T_{ij} is the transmission coefficient through the potential barrier between sites i and j, separated by the distance R_{ij}; $\Delta\epsilon = \epsilon_j + e\varphi_j - \epsilon_i - e\varphi_i$ indicates the energy difference between the initial and final states, ϵ_i and ϵ_j being the intrinsic energy levels of traps i and j, φ_i and φ_j being the values of the electric potential at the two considered sites. In the original formulation [8] the transmission coefficient T_{ij} does not depend upon electric field. However such an assumption is not realistic for a non-negligible shift of the energy barrier between the two traps due to electrostatic potential, as in the case at hand. Taking into account the effect of the electric field on the barrier [9], T_{ij} has been assumed to be

$$T_{ij} \propto e^{-2\alpha R_{ij}}, \qquad \alpha^2 = \alpha_0^2 - \frac{m_0 e \beta}{\hbar^2}|\phi_i - \phi_j|. \qquad (2)$$

In Eq. (2) α_0 is the inverse of a characteristic tunnelling distance, m_0 the free-electron mass and β a phenomenological parameter. We report in Fig. 1 the $J(V)$ curve ($J = I/\sigma$ being the current
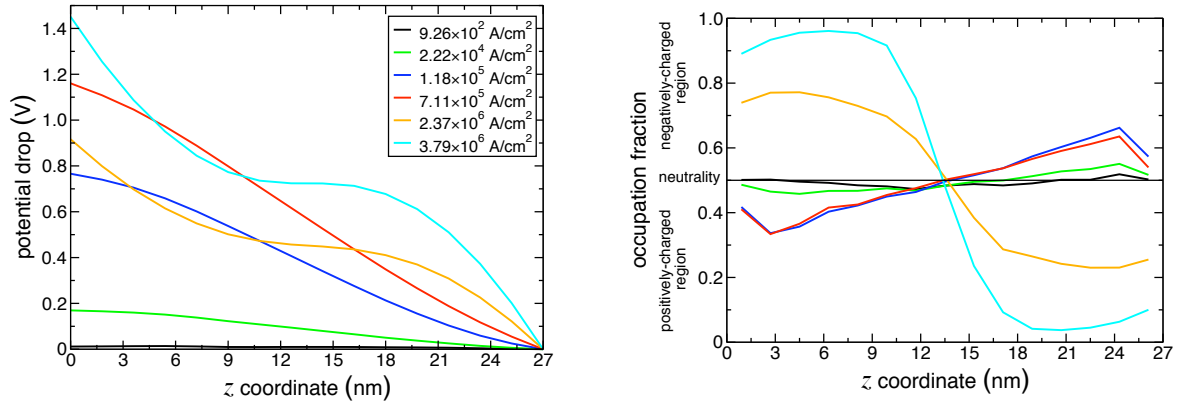

Figure 2. Left: potential profile inside the device. Each line refers to a different applied current density indicated in the legend box. Electrons enter the device from the right contact. Right: trap occupation fraction with respect to the axial coordinate of the device.

density) of the simulated device, obtained by tuning the parameters on experimental data [2]. The voltage values have been calculated as averages of the final output over 192 independent simulations. The typical features of the electric conduction in a-GST are found: a subthreshold region characterized by an Ohmic part at the lowest currents, a subsequent exponential regime, and a negative differential-resistance region. where the potential difference between contacts is reduced at increasing currents. The behavior exhibited by the upper part of the curve indicates the existence of a limiting current for the simulated model and suggests also that a different transport process like band conduction, not considered in the present analysis, must set in to sustain the prescribed current.

The outcome of the model can be interpreted from a microscopic viewpoint in terms of the trap-occupation fraction along the device and the internal electric potential profile (Fig. 2). In the subthreshold region the occupation fraction is almost constant and close to the neutrality value of 0.5, and the potential drop between electrodes is linear. For current densities larger than 10^5 A/cm^2 the hopping process is not efficient enough in transferring carriers from GST region to the collecting contact and charges tend to accumulate in the region close to the drain contact. This implies that a counterfield adds to the field generated by the two contacts. A further increase of the current enhances such effect and produces the feed-back effect necessary for the S-shape of the $J(V)$ characteristics. In fact, the traps close to the emitting contact are emptied with high rates and carriers are transferred close to the collecting contact, giving this way origin to a step-shaped profile for the trap-occupation fraction. This behavior can also be demonstrated analytically and is of fundamental importance for the occurrence of the snap-back effect.

Fig. 4 shows the probability distribution of the number of hops needed to transfer a carrier from the emitting to collecting contact, for the $I(V)$ characteristics displayed in Fig. 3. It is worth noting how at low currents the carriers emitted from one contact must hop many times to reach the drain, whilst at higher currents only a small number of hops is required. Such a behavior is related to the increase of the internal electric field that lowers the energy barriers between the traps. As a net effect, carriers are transferred from one contact to the other one by means of few long-range transitions, which are responsible for the snap-back effect. As the threshold-switching region is approached, carriers can tunnel across half the device (or more), thus enhancing the formation of opposite charge domains close to the contacts. Furthermore,

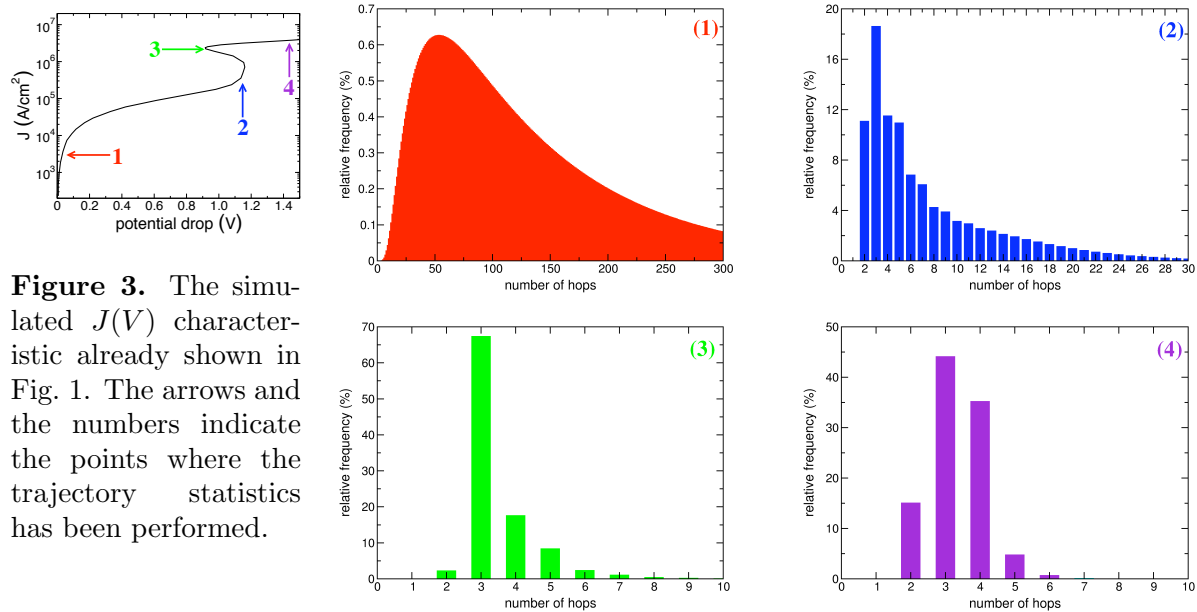the microscopic analysis of the transport process does not show evidences of carrier preferred pathways.

Figure 3. The simulated $J(V)$ characteristic already shown in Fig. 1. The arrows and the numbers indicate the points where the trajectory statistics has been performed.

Figure 4. Number of hops needed to transfer a carrier from one contact to the other. Each graph refers to a different applied current density J, indicated by the arrows and the numbers in Fig. 3. The simulated device has a cross section of 900 nm^2 and a lenght of 30 nm.

3. Conclusions

We have investigated the charge transport across a a device made of a nanometric layer of a-GST sandwiched between two metal contacts by means of a microscopic particle description. The mechanisms ruling the threshold switching have been investigated. Our result shows that the snap-back effect is related to the formation of domains of charges that modify the potential profile within the device, allowing, in turn, for higher currents to be sustained with a smaller potential drop between contacts.

Acknowledgments

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