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Modeling the Dynamic Self-Heating of PCM

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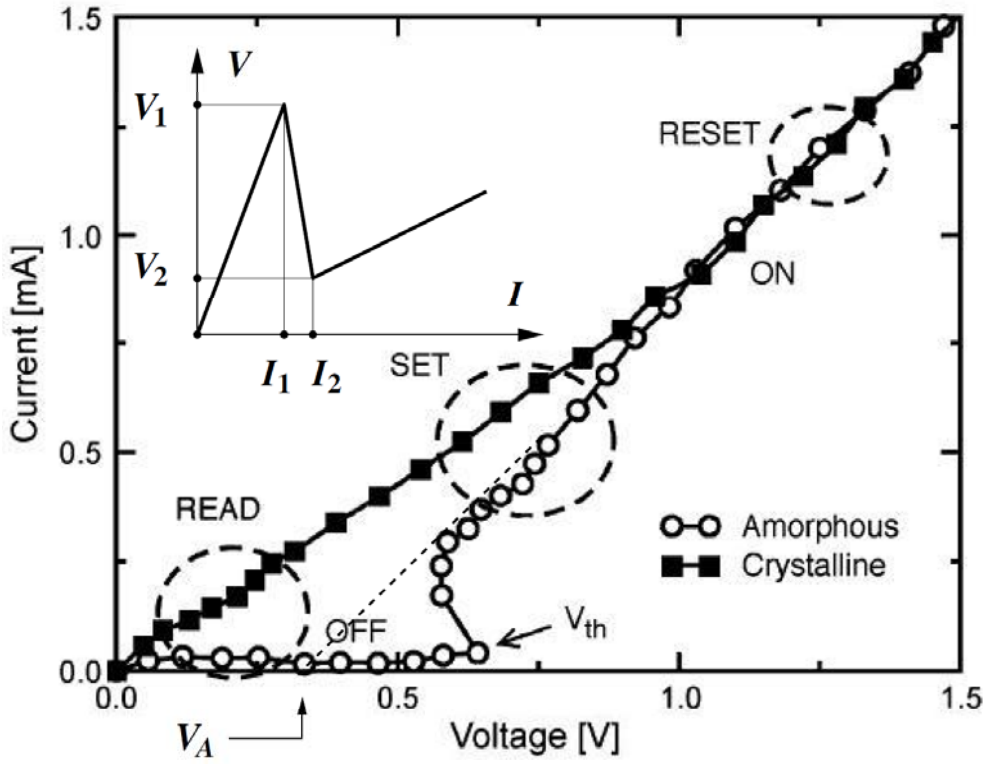
Outline

- Motivations and introduction.
- Heating induced by the dynamic measurement.
- Qualitative explanation – Quantitative approach.
- Model – Part a), b), c), d).
- Results.
- Conclusions.

Motivations

The **dynamic scheme** for extracting parameters of the phase-change memories is examined.



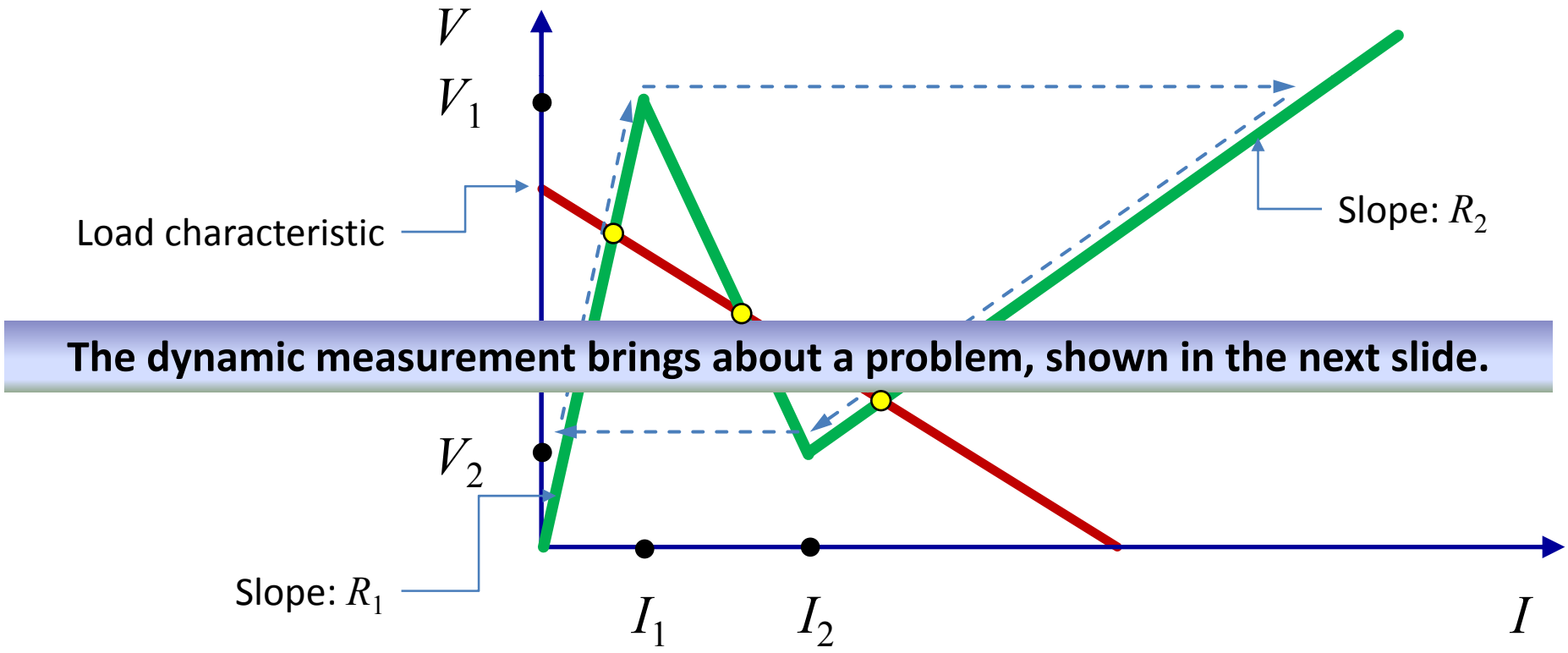
Some of the amorphous chalcogenide materials exhibit a transition **from a highly resistive to a conductive state**, characterized by a voltage snap-back. [Ovshinsky, PRL **21** (1968); Kau et al., Proc. IEDM09 (2009)].

Thanks to this property they can suitably be exploited for manufacturing **phase-change memory devices**.

Unfortunately, the static setup makes the measurements quite complicated, due to parasitic effects and the need of a current generator.

Introduction

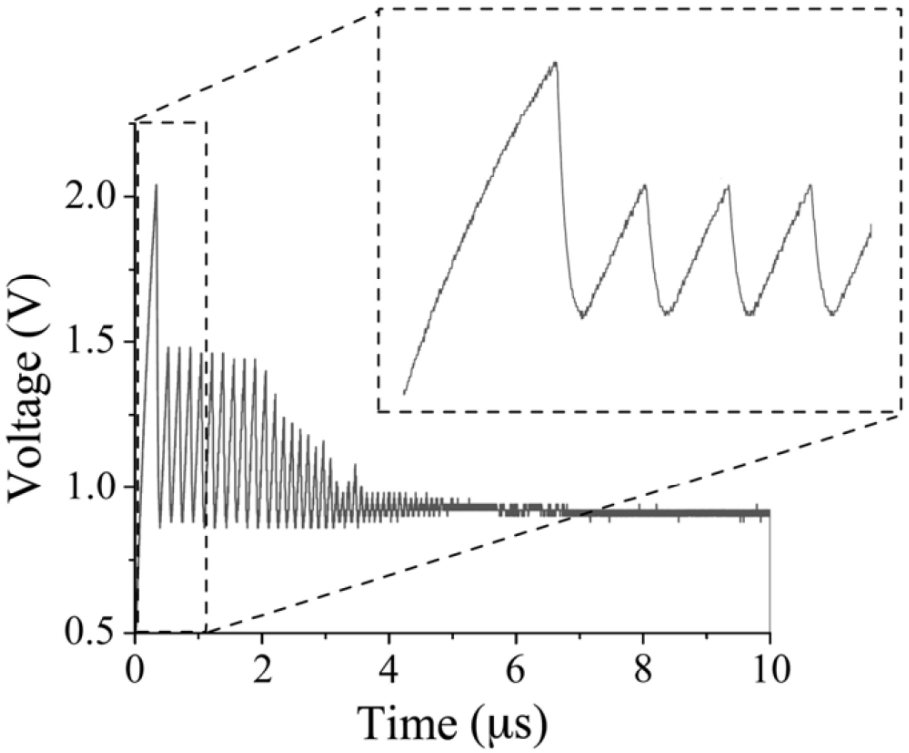
- A more effective approach to measuring the electrical characteristics is that of exploiting the **intrinsic instability** due to the negative differential-resistance branch of the PCM curve.
- Basing on this observation one arranges a **dynamic-measurement setup**.
- In this setup the characteristic of the external load intersects that of the PCM in the negative resistance branch, so that **the circuit is forced to oscillate**.



The dynamic measurement brings about a problem, shown in the next slide.

Effects of heating

- The **heating** produced by the dynamic measurement determines **a partial crystallization** of the material.
- The consequent **increase in conductivity** modifies, and possibly extinguishes, the oscillations (the figure is taken from [M. Nardone, V. G. Karpov, I. V. Karpov, *Relaxation oscillations in chalcogenide phase change memory,* J. Appl. Phys. **107**, 054519 (2010)]).

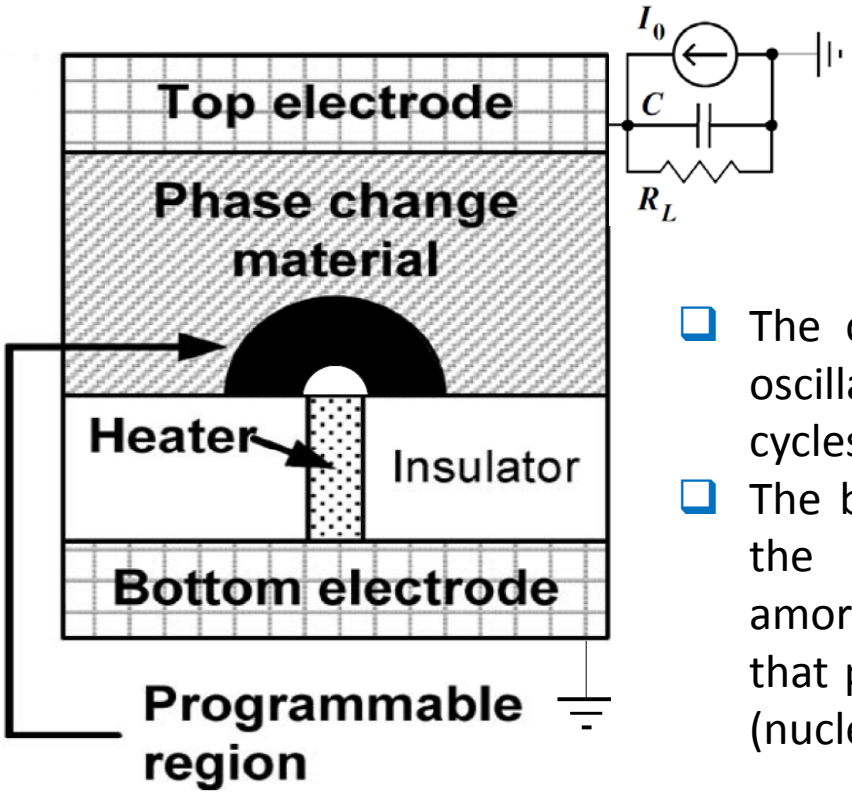


The figure shows the typical pattern of the oscillatory regime:

1. The first oscillation has a larger peak.
2. Oscillations with a stable amplitude follow.
3. Then, the amplitude of the oscillations starts to decay.

Qualitative explanation

- The strong decrease in amplitude from the first peak to the next ones is explained by the sudden crystallization of a finite portion (the **white half sphere** right above the heater) due to the concentration of the current flow-lines.
- The heater is much narrower than the amorphous region (black area), and the temperature is the highest because the whole device is still amorphous.



The figure is adapted from [H.-S. P. Wong, S. Raoux, S. Kim, J. Liang, J.P. Reifenberg, B. Rajendran, M. Asheghi, K.E. Goodson, *Phase Change Memory,* Proc. of the IEEE **98**, 12, pp. 2201–2227 (2010)].

- The conspicuous crystallization occurring in the first oscillation **leaves a smaller resistance** for the next cycles.
- The behavior from the second peak on is ascribed to the **decrease in the remaining volume** of the amorphous phase due to rapid heating and quenching, that produces the formation of small crystalline nuclei (nucleation).

Quantitative approach

The description of the oscillations must include a time-dependent thermal analysis along with the modeling of nucleation. Specifically, the following aspects must be addressed simultaneously:

a) The behavior of a non-linear circuit embedding a negative differential-resistance branch whose properties depend on time.
b) The thermal analysis of the circuit to find the time dependence of the PCM temperature.
c) The time dependence of the crystallization of a part of the PCM volume.
d) The resistivity change of the PCM and its feedback on the shape of the N-shaped characteristic.

A comprehensive modeling of the above events is carried out in the next pages.

Model — Part a)

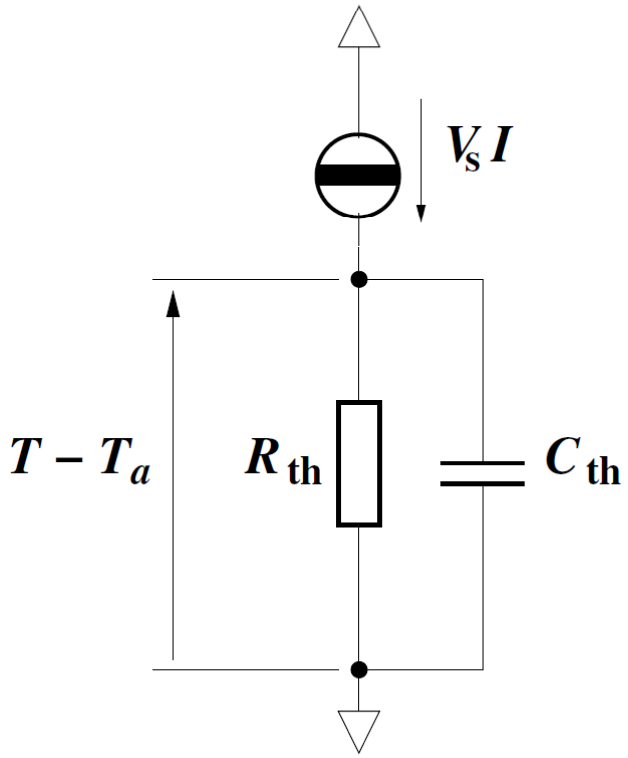
- The device under investigation is described as the **series** of an **intrinsic part** (the PCM), bearing the N-shaped characteristic, and a **constant resistance** R_S due to the heater, crystalline cap, and upper contact.
- The bias parameters are the constant current I_0 and a parallel resistance R_L.
- The oscillatory regime is sustained by a parasitic capacitance C.

- **The experimental datum** is the voltage $V(t)$ across the PCM-R_S series.
- The functioning of the **circuit** is described by the two coupled equations:

$$V = R_S I + V_S(I)\,, \qquad I = I_0 - V/R_L - C\,\mathrm{d}V/\mathrm{d}t\,.$$

- The branches of the oscillation's limit cycle in the I,V plane are determined essentially by the two points (I_1,V_1), (I_2,V_2) enclosing the negative-resistance branch.
- Among the parameters, R_S, C, I_1, I_2 are **constant**, while V_1, V_2 **change** with time because of the progressive crystallization of the material.

Model — Part b)



- The time dependence of the PCM **temperature** T is found by solving the equivalent thermal circuit [D. Ventrice, P. Fantini, A. Redaelli, A. Pirovano, A. Benvenuti, E. Pellizzer, *A Phase Change Memory Compact Model for Multilevel Applications,* IEEE Electron Device Letters **28**, 973–975 (2007)].
- The circuit, whose equation is shown below, is driven by the power $V_S I$.

$$\mathrm{d}T/\mathrm{d}t + (T - T_a)/\tau_{\mathrm{th}} = V_S\, I/C_{\mathrm{th}}$$

Here T_a is the ambient temperature and $\tau_{\mathrm{th}} = R_{\mathrm{th}} C_{\mathrm{th}}$, with R_{th}, C_{th} the thermal resistance and capacitance, respectively.

Model — Part c)

- Crystallization starts with the formation of small unstable clusters of the new phase (**nucleation process**; a "nucleus" is the minimum-size volume that crystallizes).
- Eventually some clusters reach a critical radius beyond which they are stable, so that they can grow rather than dissolve (**growth process**).
- Let g be the number of nuclei in a cluster, $N_g(t)$ the concentration at time t of clusters made of g nuclei, and $P_g = N_g / \Sigma_g N_g$ the **probability** that a cluster is made of g nuclei.

The dynamic model for the crystallization phase transformation is taken from [E. M. Wright, P. K. Khulbe, M. Mansuripur, *Dynamic theory of crystallization in* $Ge_2Sb_{2.3}Te_2$ *phase-change optical recording media,* Appl. Optics **39**, 6695 (2000)] and reads (with $\sum_{g=1}^{g_{max}} P_g = 1$)

$$dP_1/dt = r(t) - (C_1 P_1 - E_2 P_2) - r(t) P_1 ,$$

$$dP_g/dt = C_{g-1} P_{g-1} - E_g P_g - C_g P_g + E_{g+1} P_{g+1} ,$$

$g = 2, 3, \ldots$, with C_g the **condensation rate** (the number per unit time of g-sized clusters that grow by one nucleus), E_g the **evaporation rate** (the number per unit time of g-sized clusters from which one nucleus dissolves), and r the **generation** rate of the nuclei.

Part c) of the model has 3 fitting parameters.

Model — Part d.1)

- During the oscillations the temperature increases beyond the **glass temperature** T_g. As a portion of the volume crystallizes, the dissipated power decreases due to the decrease in resistance.
- However, the input power is still sufficient to continue the crystallization process. In parallel, the **amplitude of the oscillations decays** due to the decreasing resistance.
- When the whole device is in the amorphous phase the positive slopes are either R_1 or R_2 depending on the current.
- If the heating and quenching process ended up in the crystallization of the whole volume, the two resistances R_1, R_2 would transform into the resistance R_c of a volume of crystalline material equal to that of the original device.

When only **part of the volume** is crystallized, the expressions of the two positive-slope branches become

$$V = (R_S + r_{1(2)})\, I\,, \quad r_{1(2)} = (1-\lambda)\; R_{1(2)} + R_c\, \lambda\,,$$

where $0 \leq \lambda(t) = (H - H_{\mathrm{am}}) \,/\, H \leq 1$ is the fraction of the crystallized volume, with $H_{\mathrm{am}}(t)$ the length of the PCM that has not crystallized yet and H the initial length. The value of $\lambda(t)$ is extracted from the nucleation equations.

Model — Part d.2)

- The thermal resistance of the thermal circuit at t is calculated from

$$R_{\rm th} = (1-\lambda)\, R_{\rm th}^{\rm am} + R_{\rm th}^{\rm cr}\, \lambda\,, \quad A\, R_{\rm th}^{\rm am(cr)} = H\, \rho_{\rm th}^{\rm am(cr)}$$

where A is the PCM cross-sectional area, $\rho_{\rm th}$ the thermal resistivity, and the suffix "am" ("cr") refers to the amorphous (crystalline) phase.

- The values used here are $H = 100$ nm, $A = 180 \times 180$ nm^2, $\rho^{\rm am}{}_{\rm th} = 500$ KcmW^{-1}, *and* $\rho^{\rm cr}{}_{\rm th} = 200$ KcmW^{-1} [A. Pirovano, A. L. Lacaita, A. Benvenuti, F. Pellizzer, S. Hudgens, and R. Bez, *Scaling Analysis of Phase-Change Memory Technology*, in IEDM Tech. Dig., 2009, pp. 699-702].
- The thermal capacitance does not depend on the material's phase and reads $C_{\rm th} = c_p H A$, $c_p = 1.25$ Jcm^{-3}K^{-1}.

- The time dependence of V_1, V_2 changes the form of the N-shaped curve.
- The oscillation continues as long as the characteristic of the external load intersects that of the PCM in the negative-resistance branch.

Model — Summary

To summarize, the model is made of the following equations, that form a set non-linear, coupled, differential or algebraic equations, supplemented with the **constitutive equations** for the coefficients r, C_g and E_g :

$$V = R_S I + V_S(I)\,, \qquad I = I_0 - V/R_L - C\,\mathrm{d}V/\mathrm{d}t\,.$$

$$\mathrm{d}T/\mathrm{d}t + (T - T_a)/\tau_{\mathrm{th}} = V_S\, I/C_{\mathrm{th}}$$

$$\mathrm{d}P_1/\mathrm{d}t = r(t) - (C_1\, P_1 - E_2\, P_2) - r(t)\, P_1\,,$$

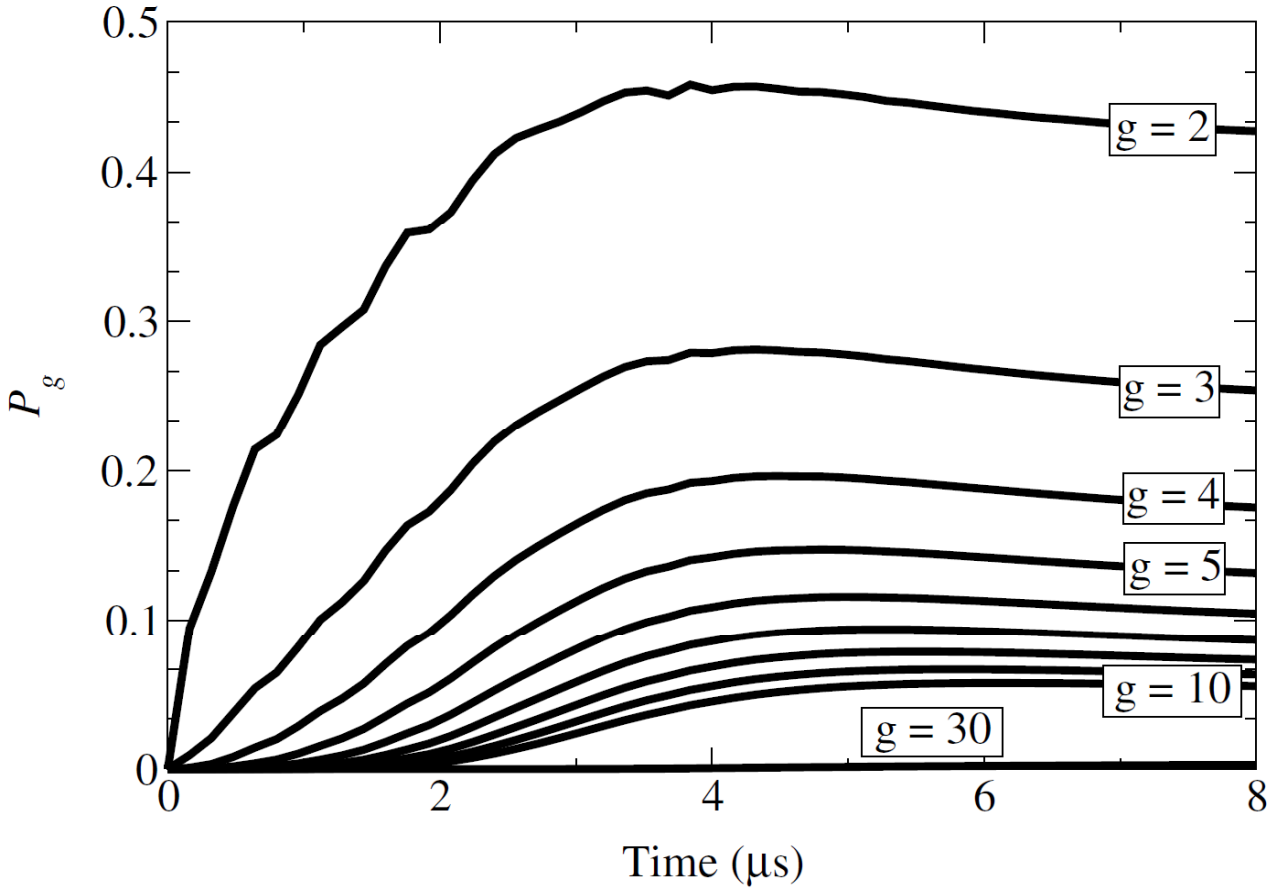
$$\mathrm{d}P_g/\mathrm{d}t = C_{g-1}\, P_{g-1} - E_g\, P_g - C_g\, P_g + E_{g+1}\, P_{g+1}\,,$$

$$V = (R_S + r_{1(2)})\, I\,, \quad r_{1(2)} = (1-\lambda)\, R_{1(2)} + R_c\, \lambda\,,$$

$$R_{\mathrm{th}} = (1-\lambda)\, R_{\mathrm{th}}^{\mathrm{am}} + R_{\mathrm{th}}^{\mathrm{cr}}\, \lambda\,, \quad A\, R_{\mathrm{th}}^{\mathrm{am(cr)}} = H\, \rho_{\mathrm{th}}^{\mathrm{am(cr)}}$$

The differential part entails a non-trivial **open integration**, that is tackled by the integral-equation method of [M. Rudan, A. Gnudi, E. Gnani, S. Reggiani, G. Baccarani, *Improving the Accuracy of the Schrödinger-Poisson Solution in CNWs and CNTs*, Proc. SISPAD 2010, 307–310 (2010)].

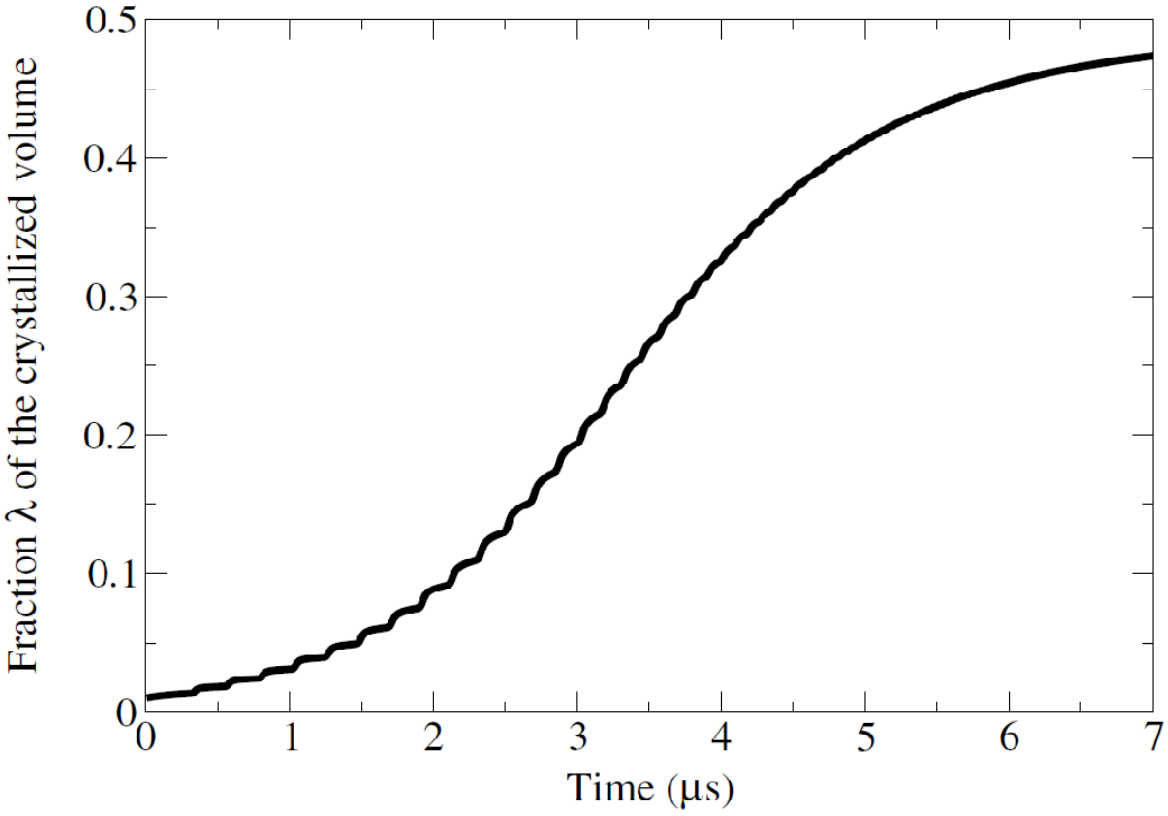
Time evolution of the clusters



Probability P_g that a cluster is made of g nuclei as a function of time. Each probability tends to saturate with *t*. The probability of relatively large clusters (for example, $g = 30$ or larger) is negligible for the device investigated here.

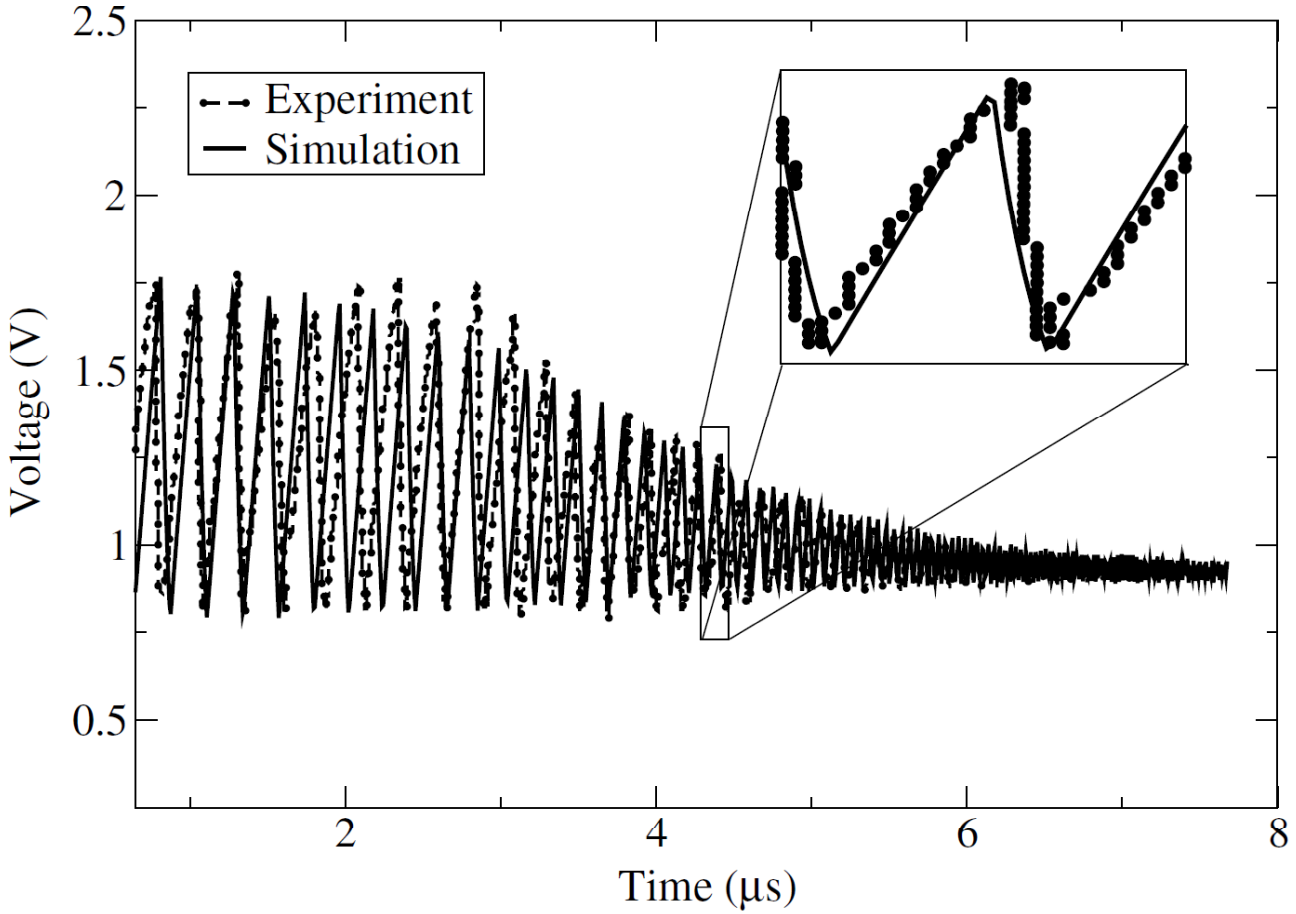
Crystallization vs time

- The figure shows the fraction λ of the crystallized volume as a function of time.
- The increase in λ corresponds to the decay of the peaks, and is relatively slower than the oscillation period.
- A 1 ps discretization time coupled with a 5th order integral-equation method gave the numerical scheme the required accuracy.
- The temperature of the material never exceeded the melting temperature T_m.



Comparison with experiments — 1

The outcome of the model has been compared with the experiments of [M. Nardone, V. G. Karpov, I. V. Karpov, *Relaxation oscillations in chalcogenide phase change memory*, J. Appl. Phys. **107**, 054519 (2010)].



- The experimental curve has been converted into a discrete set to make the fitting of parameters possible.
- The first, larger peak is related to a three-dimensional effect that is not included in the present model.
- The comparison has been carried out starting from the second peak.

Comparison with experiments — 2

- The model captures at the same time the period of the oscillations and the decay of the voltage peaks due to the progressive crystallization of the material.
- Due to the voltage decay the crystallization conditions become weaker and weaker, and the fraction of crystallized material tends to saturate as shown earlier in the figure.
- In the experiments considered here, when such a saturation occurs the characteristic of the external load still intersects that of the PCM in the negative differential-resistance branch (the oscillations stabilize).
- In other cases (not shown) the deformation of the PCM characteristic shifts the bias point out of the characteristic of the external load, and the oscillations eventually come to an end.

Conclusions

- A comprehensive model for the oscillation decay in PCM devices due to the progressive crystallization of the material has been given.
- The equations proposed here are able to capture the experimentally-observed macroscopic behavior of the device.
- With the aid of a thermal circuit monitoring the PCM temperature and the time spent in the glass-melting temperature range, it is possible to evaluate the state of the cell under different experimental conditions.
- A number of parameters appearing in the non-equilibrium nucleation theory have been determined by a fitting procedure.

The method makes it possible to extract the parameters that describe the N-shaped characteristic, including their heating-induced time variation, that are of a paramount importance in the design of PCM.

Thank You
for Your Attention!