THE PUBLISHING HOUSE
OF THE ROMANIAN ACADEMY

PROCEEDINGS OF THE ROMANIAN ACADEMY, Series A,
Volume 10, Number 3/2009, pp. 000–000

PHASE CHANGE MATERIALS: CHEMICAL BONDING AND STRUCTURAL PROPERTIES

AlinVELEA [a,b], Mihai POPESCU [a,b]

a) National Institute of Materials Physics, 077125-Bucharest-Magurele, Ilfov, Atomistilor str. 1, P. O. Box MG. 7, Romania
b) "Horia Hulubei" Foundation, Bucharest-Magurele, P. O. Box Mg. 5, Romania
Corresponding author: velea@infim.ro

The phase change materials are the most important materials in the class of chalcogenides (combination of chalcogens (S, Se and Te) with metalloids or metals). The outstanding property of these materials is the switching from a high electrical resistivity state to low electrical resistivity state and back under a moderate voltage. The thin film materials are used in computer memories, CD and DVD devices with performing speed and storage capacity. We have studied several thin solid films made of Ge-Sb-Te in order to assess the switching quality of different compositions. In order to systemize the whole class of chalcogenide phase change materials we have investigated the correlation between different crystallo-chemical parameters and the ionicity of the elements. Binary and ternary compounds are distributed into several distinct groups. The most favorable phase change materials are situated in a specific range of mean ionicity and mean glass formation ability. The results give the possibility to design new compositions with better switching properties.

Key words: Phase change materials; Switching mechanism; GeSbTe.

1. INTRODUCTION

Switching effect in amorphous materials has been discovered by Ovshinsky in 1968 [1]. The effect consists in the reversible modification of the resistance of a thin film under the influence of a short electrical pulse applied to the material. Figure 1 illustrates the effect.

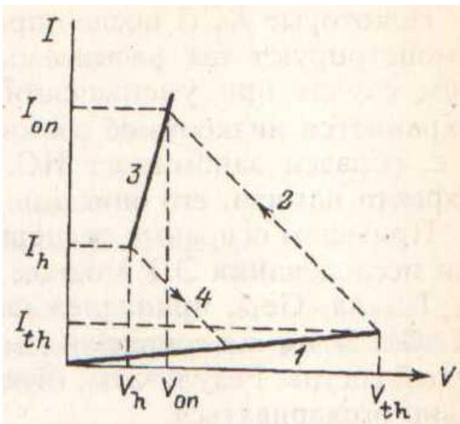

Figure 1. The switching effect

Data on the switching parameters have been published in literature [2-4] and some of them have been used in this article.

2. CRYSTALLO-CHEMICAL PARAMETERS

In order to relate the switching parameters on the crystallo-chemical characteristics of a chalcogenide material we introduced two parameters: the reduced ionicity (RI) and the Glass ability (GA). $RI = \frac{I_1}{\eta}$ is the mean ionicity of the compound divided by η, the weighted mean of the inverse of the orbital radius in the compound or alloy. Glass ability is defined by $GA = \frac{\overline{n}\overline{k}}{\overline{Z}}$ where $\overline{n}$ is the mean value of the last orbital occupied by electrons, $\overline{k}$ is the mean coordination number and $\overline{Z}$ is the mean of the atomic number of atoms entering into the composition of the material.

As switching parameters were taken into account: the threshold potential (V_{th}) for switching, the resistivity of the material and the number of cycles supported by a given material.

3.RESULTS

3.1. Ge – Sb – Te system

One of the most important chalcogenide systems used in switching is Ge – Sb – Te. Tellurium seems to be an essential element that ensures the rapidity, reversibility and stability of the switching along many cycles. The ternary phase diagram is shown in Figure 2. The switching compositions, well studied, are represented by black dots.

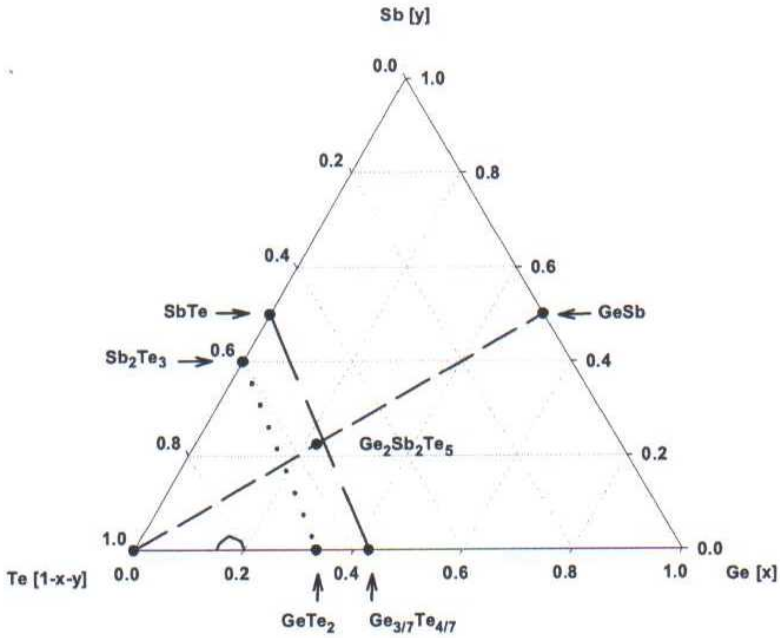

Figure 2. Phase diagram of Ge – Sb – Te

We have transformed the usual phase diagram in a special one related to crystallo-chemical parameter RI. (Figure 3). During switching the structural properties of the material changes from the crystalline state to the amorphous state. In this system the most important modification is the change in coordination from octahedral one (as demonstrated in $GeAs_2Te_4$ to the natural coordination of every type of atom (4 for Ge, 3 for Sb and 3 for Te). As a consequence, the points situated in the crystallo-chemical triangle shift to various positions as a function of the quality of switching. A careful analysis of the switching material is necessary in order to get the structural data.

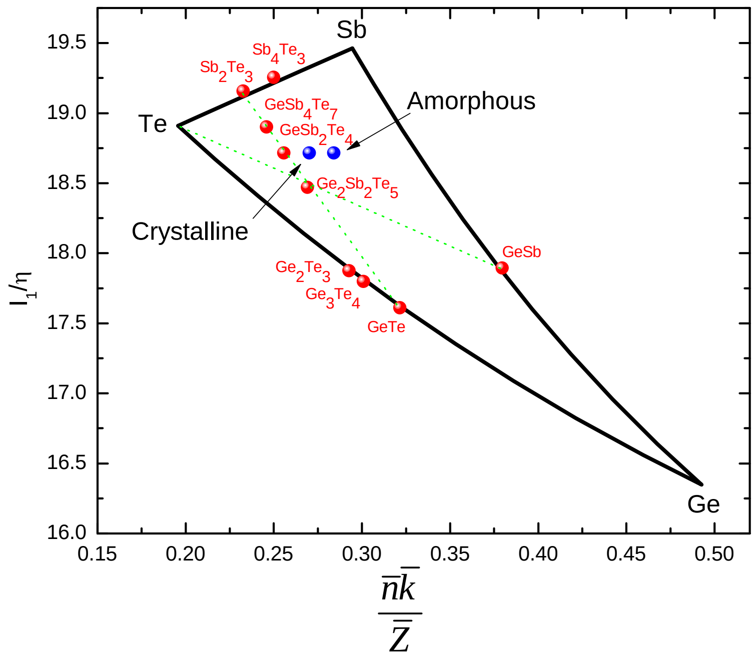

Figure 3 The new phase diagram based on the crystallo-chemical parameters

3.2. As – Se – Te system

We have analyzed the switching in the system As_2Se_3-As_2Te_3 as a function of the parameters: GA and RI. Figs. 4 - 6 show the results. The correlation between the two parameters GA and RI is linear. The correlation of the ionicity with threshold voltage and resistivity is also evidenced. The threshold voltage [5] decreases with the ionicity of the material. The resistivity decreases, too, with ionicity. (Fig. 5). The electrical conductivity is also correlated with the reduced ionicity (Fig. 6).

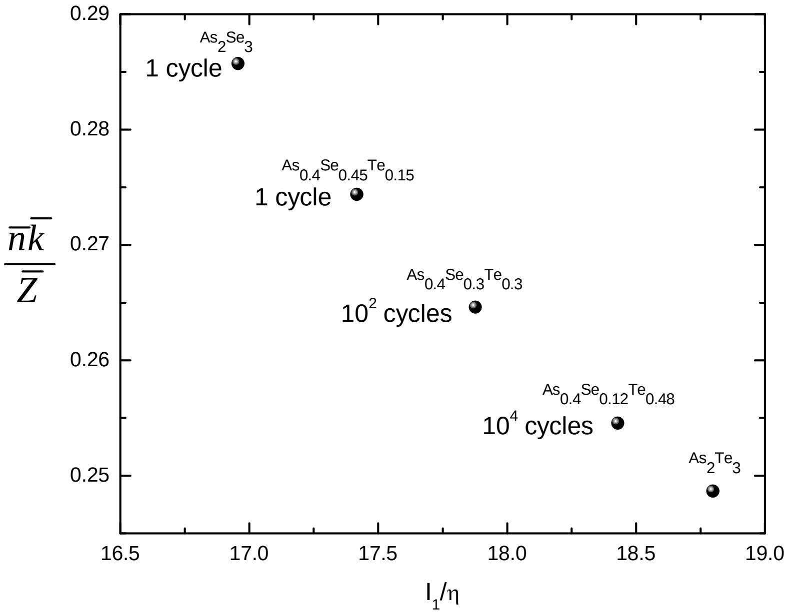

Figure 4. Glass ability as a function of reduced ionicity

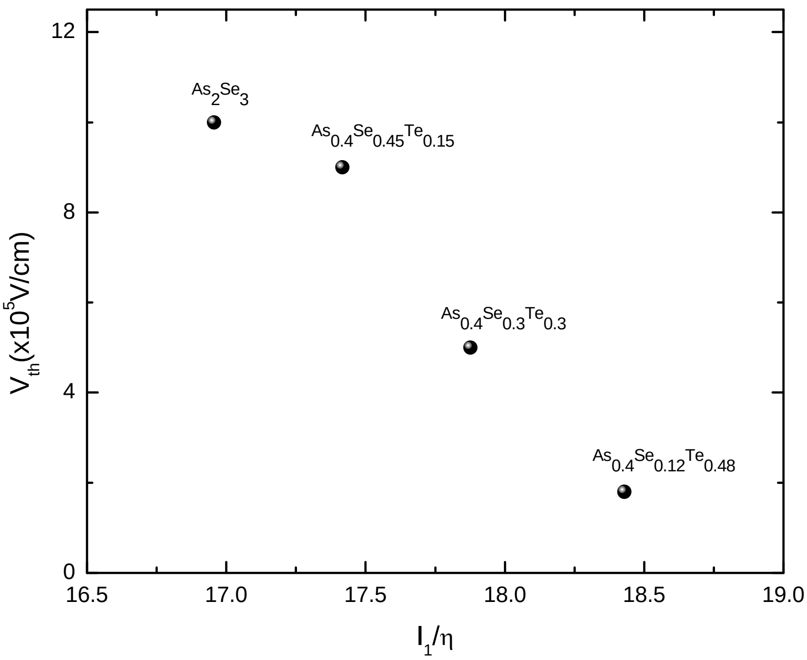

Figure 5. Threshold voltage as a function of reduced ionicity

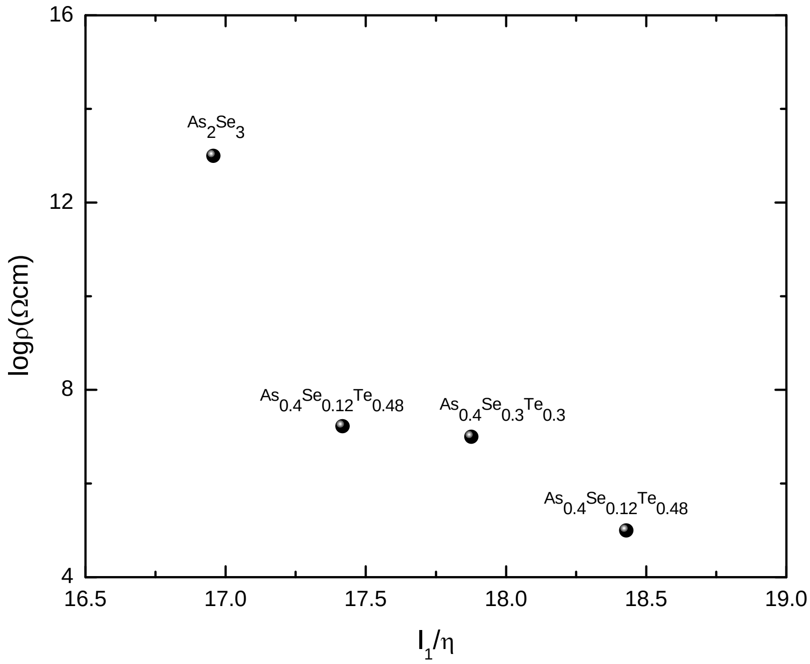

Figure 6. Conductivity as a function of reduced ionicity

3.3. Ge – As – Te – Se system

Similar correlations are found in the system Ge-As-Te with Selenium (Fig. 7, 8 and 9). All the graphs speak in favour of a strong dependence of the switching quality on the ionicity of the material. The data and the switching parameters are from [5].

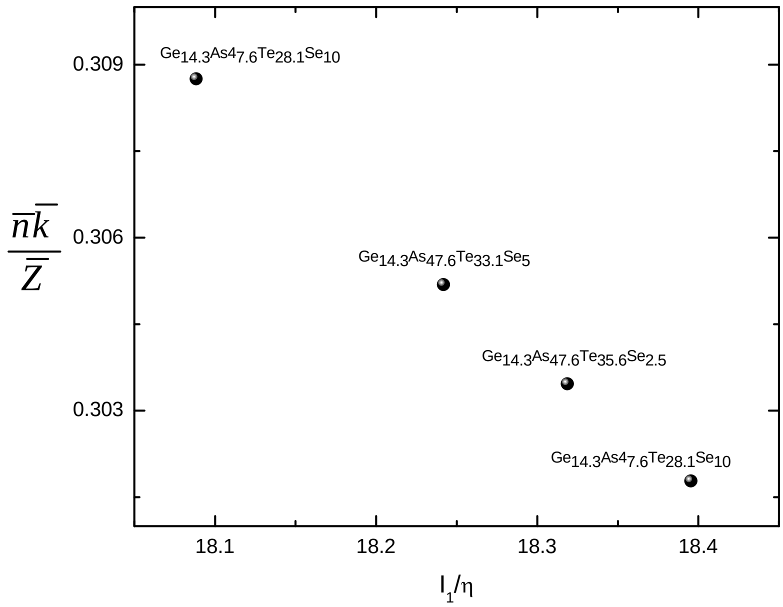

Figure 7. Glass ability as a function of reduced ionicity for a quaternary phase change system : Ge - As -Te + Se

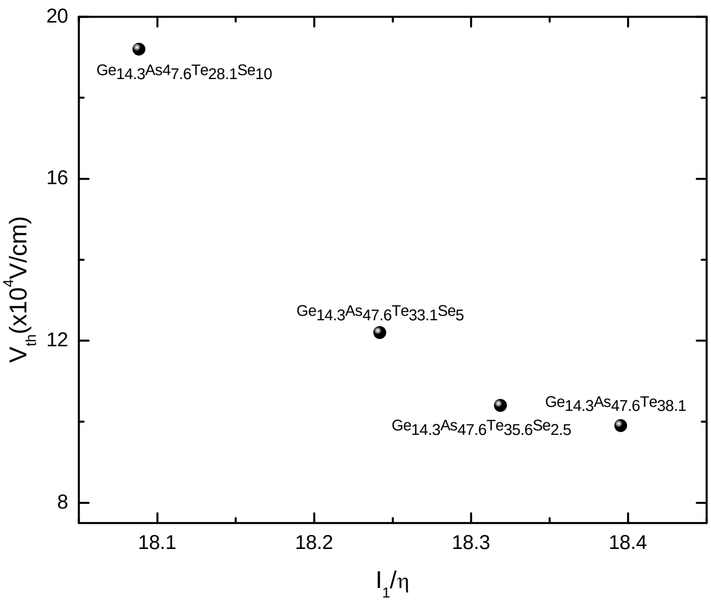

Figure 8. Threshold voltage as a function of reduced ionicity for the system Ge – As – Te + Se

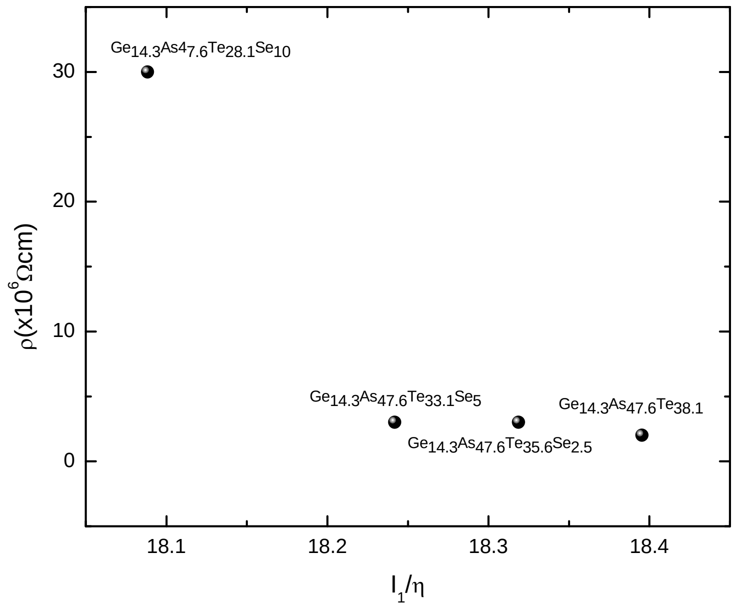

Figure 9. Resistivity versus reduced ionicity in the system Ge – As – Te – Se

3.4. Ge – Si – As – Te system

The quaternary system behaves similarly. Essentially the resistivity increases with the mean ionicity of the material

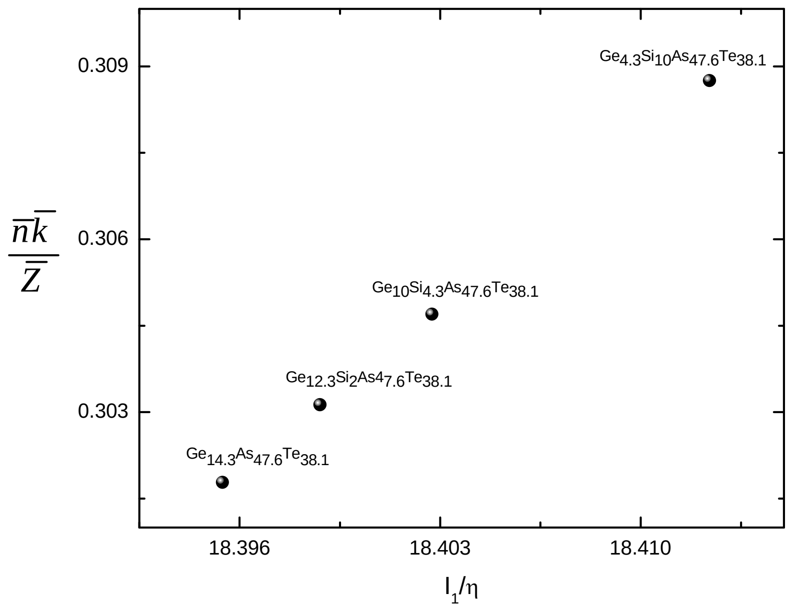

Figure 10. Glass ability versus reduced ionicity for Ge – As – Te with Si

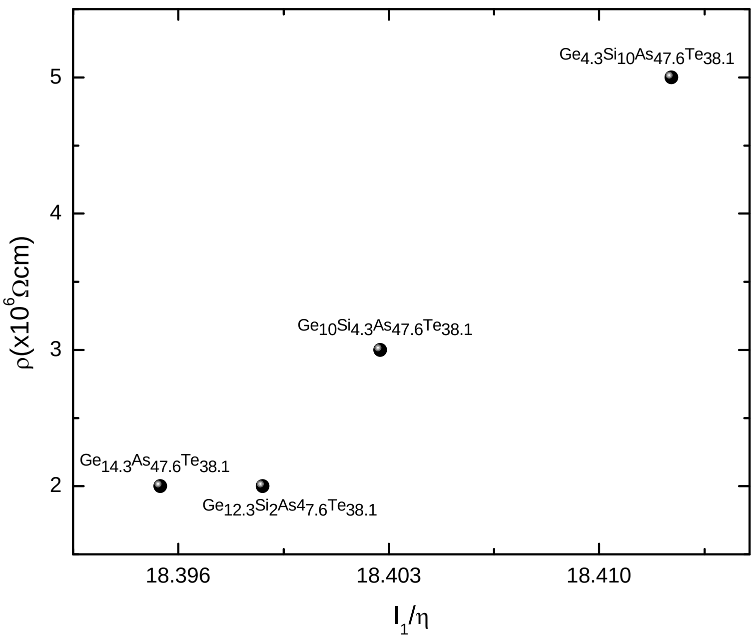

Figure 11. Resistivity versus reduced ionicity for Ge – As – Te + Si

4. CONCLUSIONS

The properties of the switching chalcogenide materials depends strongly on the chemical characteristic of the material. The ionicity is one of the most important factors. The glass ability is also important. We cdan conclude that materials which easily form glasses exhibit better switching properties.

REFERENCES

1. OVSHINSKY S. R., *Reversible Electrical Switching Phenomena in Disordered Structures*, Phys. Rev. Lett. 21, p. 1450, 1968
2. MATSUNGA T., YAMADA N., *Structural investigation of $GeSb_2Te_4$: A high-speed phase-change material*, Phys. Rev. B 69, 104111, 2004.
3. FRITZSCHE H., *Why are chalcogenide glasses the materials of choice for Ovonic switching devices?*, J. Phys. Chem. Solids, 68, p.878-882, 2007.
4. LENCER D., SALIGNA M., GRABOWSKI B., HICKEL T., NEUGEBAUER J., WUTTIG M., *A map for phase-change materials*, Nat. Mat, Vol. 7, p. 972-977, 2008.
5. TSENDIN C. D., *Electronic phenomena in chalcogenide glassy semiconductors* (Russian), Ed. Nauka, Sankt-Petersburg, 1996.

Receiving June 8, 2009