Ab-initio simulation of resistive memory based on GeTe-Sb_2Te_3 alloys

Zalevskyi D.V., Balabai R.M.

Kryvyi Rih State Pedagogical University, 54 Gagarina Ave., Kryvyi Rih, 50086, Ukraine.

denys.zalevski@gmail.com, balabai@i.ua

1. INTRODUCTION AND FORMULATION OF THE PROBLEM

Currently, memory devices based on materials with phase change (PCM) are being actively developed [1].

Phase change materials have a unique combination of properties, which makes them promising candidates as carriers in random access memory devices with phase change (PCRAM) [2]. A material with a phase change is one that exists in at least two phases with extremely different optical or electrical properties and can be repeatedly and quickly switched between these phases. In recent years, Ge-Sb-Te (GST) alloys have been studied in detail as the main candidates as phase-change materials [3].

Chalcogenide semiconductors on the quasi-binary line GeTe-Sb_2Te_3 are considered to be the most promising materials for use in memory with phase change [4] due to high crystallization rate and high stability at room temperature [5].

The materials $Sb_2Ge_xTe_{3-x}$ (x = 0,1,2): Sb_2Te_3, $Sb_2Ge_1Te_2$, $Sb_2Ge_2Te_1$ are investigated in the work by the methods of electron density functional and pseudopotential from the first principles on our own program code [7].

2. METHODS OF RESEARCH

The basic states of the electron-nucleus systems were detected by means of the self-consistent solution of the Kohn-Sham equations. Electronic variables only were determined with the atomic cores fixed.

The point on the surface of potential energy in the Born-Oppenheimer approximation was determined as a minimum energy functional.

In the generally accepted formulation, minimization of the energy functional with respect to one-particle orbitals with additional orthonormal constraint on the one-particle orbitals.

In the solution of these equations, the pseudopotential formalism was used, according to which a solid is considered as a set of valence electrons and the ion cores. *Ab initio* pseudopotential is used by us.

The artificial super-lattice method was used in calculations. Therefore, in the studied atomic systems, the artificial translational symmetry was introduced by constructing of a super-lattice with a primitive rhombic cell and the atomic basis which contains the complete information about the studied system.

3. OBJECTS, RESULTS OF CALCULATION AND THEIR DISCUSSION

Our work shows the similarities and differences between chemical bonding and electronic properties between Sb_2Te_3, $Sb_2Ge_1Te_2$, $Sb_2Ge_2Te_1$ crystals.

An infinite Sb_2Te_3 crystal was formed for the calculations. When creating the atomic basis, the atoms were arranged in the form described in [6] (arrangement of atoms, organization of layers and distances between them).

Infinite crystals Sb_2Te_3, $Sb_2Ge_1Te_2$, $Sb_2Ge_2Te_1$ were created to perform the calculations. Since the calculation algorithm assumes the presence of translational symmetry in the system, a cell with parameters a = 14.77 Å, b = 12.79 Å, c = 32.24 Å was created. The choice of these parameters took into account the need to create an infinite crystal. The atomic basis for $Sb_2Ge_1Te_2$ and $Sb_2Ge_2Te_1$ crystals was realized by replacing Te atoms with Ge atoms without changing their position.

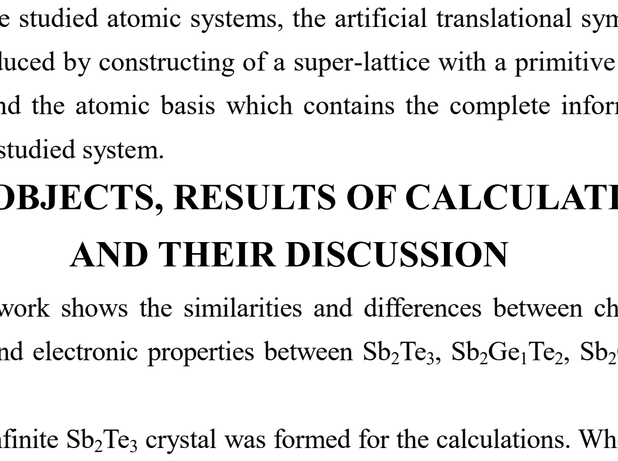

Fig. 3. Cells with atomic basis for different objects of calculation

Characteristics of model objects (Fig. 3): Object 1 - Infinite Sb_2Te_3 crystal containing 108 Te atoms and 72 Sb atoms; Object 2 - Infinite $Sb_2Ge_1Te_2$ crystal containing 72 Te atoms, 72 Sb atoms and 36 Ge atoms; Object 3 - Infinite crystal $Sb_2Ge_2Te_1$ containing 36 Te atoms, 72 Sb atoms and 72 Ge atoms;

The spatial distribution of electron density for the studied objects is shown in Fig. 4. Due to the close values of electronegativity for Sb, Te and Ge atoms, it can be stated that the type of interatomic bonds within each quintet is covalent. And between the atoms in the extreme layers of the quintets there is a Van der Waals interaction. This is confirmed by the pattern of electron density distribution.

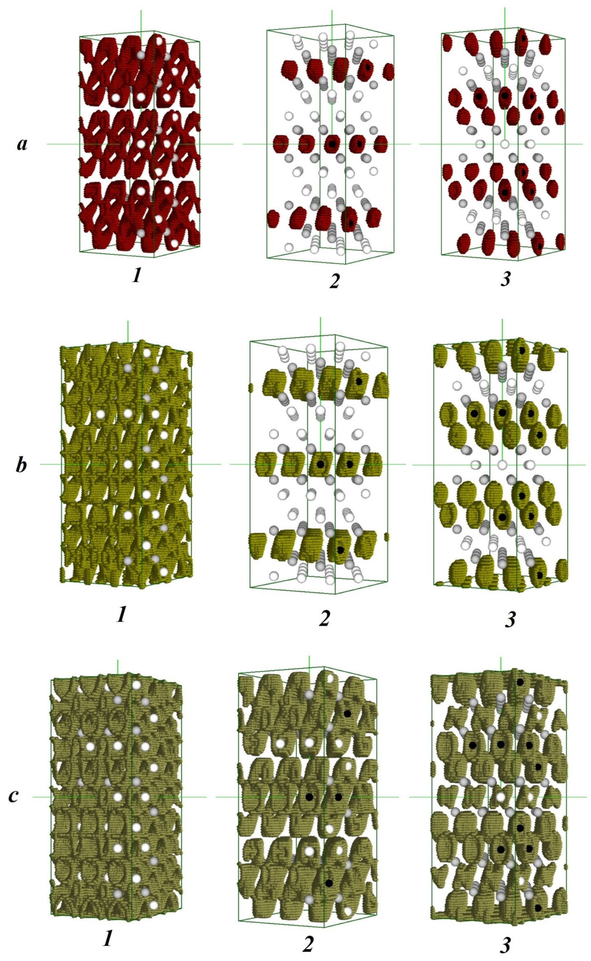

Fig. 4. Spatial distributions of valence electron density within the cell for the isovalues of 0.8-0.7 (a), 0.6-0.5 (b), 0.4-0.3 (c) from the maximum for objects 1-3

The directional covalent bonds between Sb and Te for object 1 are clearly visible. The distribution of electron density at objects 1 and 3 makes it possible to draw a conclusion about the organization of covalent bonds within quintets and Van der Waals - between quintets.

The Ge atoms in objects 2 and 3 are surrounded by a characteristic spherical electron density, which indicates that the distances between the German atoms in the calculation were larger than those required to form a covalent bond.

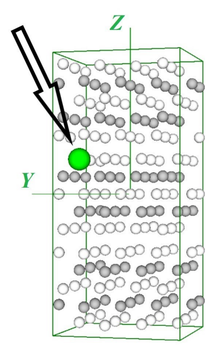

Fig. 5. The position of the atom around which the distribution of electron density was studied (the position of the atom indicated by the arrow)

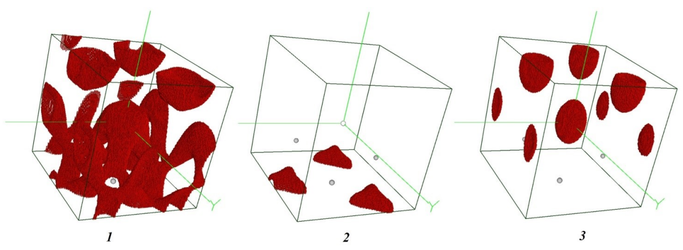

Fig. 6. The spatial distribution of the density of valence electrons near the studied atom for the isovalues of 0.8-0.7 from the maximum for objects 1-3

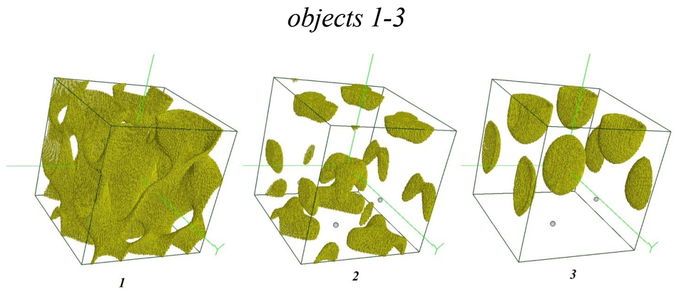

Fig. 7. The spatial distribution of the density of valence electrons near the studied atom for the isovalues of 0.6-0.5 from the maximum for objects 1-3

To study the nature of the interaction between the quintets, an atom on one of the extreme layers of the quintet (for all objects) was selected and the area around it with a radius of 3 Å was considered. Fig. 6 and 7 show the calculated spatial distributions of the electron density and their cross sections (Fig. 8) in this region. It can be seen that the change in chemical composition from object to object is reflected in the maps of the distribution of valence electron density and in the nature of the chemical bond between the quintets.

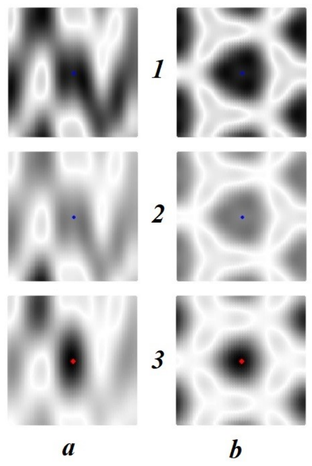

Fig. 8. Sections of spatial distributions of valence electron density within the investigated atom: a - plane (110) section for objects 1-3, b - plane (100) section for objects 1-3

When analyzing the density distribution of electronic states, certain specific features can be identified (Figs. 9, 10, 11). For objects 2, 3, in which part of the atoms are replaced by Ge atoms, the subband in the levels of which the German electrons are located is clearly visible in the organization of the valence bands. The width of the valence band for the three objects differs slightly: 45 eV for the object 1, 53 eV for the object 2, 57 eV for the object 3. We see the broadening of the valence band with increasing concentration of Ge atoms in the crystal.

As for the states in the conduction band, they appear at a small energy distance from the valence band in all objects under study. Width of this distance: 0.1 eV for object 1, 0.003 eV for object 2 and 0.03 eV for object 3.

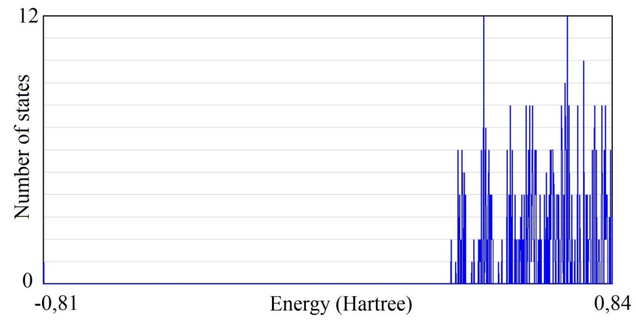

Fig. 9. Density of electronic states for object 1

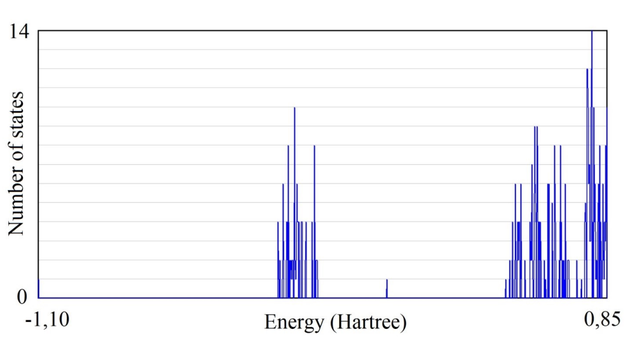

Fig. 10. Density of electronic states for object 2

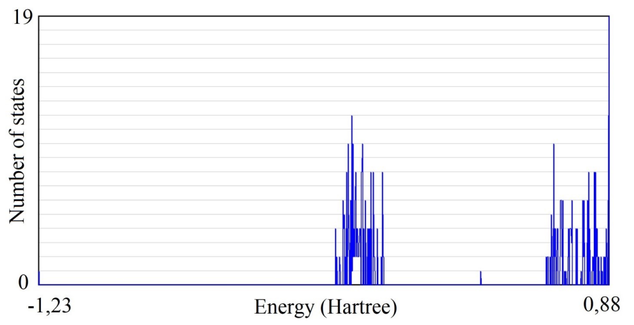

Fig. 11. Density of electronic states for object 3

4. CONCLUSIONS

Using the methods of the theory of electron density functional and pseudopotential from the first principles on the basis of own program code the characteristics of materials $Sb_2Ge_xTe_{3-x}$ (x = 0,1,2) which can act as a working layer of PCRAM are received. The spatial distribution of the density of valence electrons, the density of electronic states, the band gap for these materials are calculated.

For materials Sb_2Te_3, Sb_2GeTe_2, Sb_2Ge_2Te, there is a noticeable difference in the electron density distribution, the nature of the chemical bonds in the crystal, the organization of the band structure of the materials, and the conductive properties. Thus, for objects 2 and 3, in which part of the atoms are replaced by Ge atoms, the subband in the levels of which the electrons of Germany are located is clearly visible in the organization of the valence bands. The band gap is: 0.1 eV for object 1, 0.003 eV for object 2 and 0.03 eV for object 3. The electron density distribution indicates the presence in the quintet of interatomic bonds of the covalent type, and between atoms in the extreme layers of quintets - Van der Waals type.

5. REFERENCES

1. S. Raoux, W. Weinie, D. Ielmini. *Chem Rev.* 110, 240 (2010)
2. H.-S.P. Wong, S. Salahuddin. *Nat. Nanotechnol.* 10, 191 (2015)
3. M.A. Zidan, J.P. Strachan, W.D. Lu. *Nat. Electron.* 1, 22 (2018)
4. Q. Xia, J.J. Yang. *Nat. Mater.* 18, 309 (2019)
5. J. Feldmann, N. Youngblood, C.D. Wright, H. Bhaskaran, W.H.P. Pernice. *Nature* 569, 208 (2019)
6. T. Anderson, B. Krause. *Acta Cryst.* 30, 1307 (1974).
7. Ab initio calculation [E-resource] – Mode access to the resource: http://sites.google.com/a/kdpu.edu.ua/calculationphysics.