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INVESTIGATION OF THE PROPERTIES OF $Ge_{1-x}Sn_x$ SEMICONDUCTOR SOLID MIXING ZONE STRUCTURE

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Abstract
Currently, the fields of nanoelectronics, optoelectronics and photonics are developing rapidly. In these areas, the creation of effective working materials is an important task. Traditional Si&Ge based semiconductors are not suitable for photonics because they have an indirect energy gap.

Introduction

On the other hand, the solid mixture of $Ge_{1-x}Sn_x$ can be converted from an indirectly void to a hollow material by increasing the amount of Sn, making it a promising material for optoelectronic devices, lasers, and infrared detectors.Group IV alloys are of great interest in the way of creating silicon(Si)-compatible, direct-band gap (bandgap) materials. These materials are important for silicon-based metal oxide semiconductor technology and subsequent new electronic devices. The lack of direct bandwidth of Si and Ge materials limits their possibilities of use in optoelectronics and photonics devices, as the introduction of excess deformation is required to produce the desired optical properties.

Combining Ge and Sn elements as alloy is a promising solution to overcome the shortage of luminous emitting capacity of group IV materials.

In this master's thesis, this study investigates and analyzes the zone structure properties of a semiconductor solid mixture of Snx. Depending on the ratio of Ge (germanium) and Sn (tin) atoms, the electronic structure, energy zones, transition holes and bonding properties of the alloy were studied. Quantum-mechanical calculations based on density functional theory (DFT) were carried out by deducing the zone diagram of the mixture $Ge_{1-x}Sn_x$, the network parameters and bonding energies. The obtained results allow to evaluate the possibility of application of this material in optical and electronic devices in the infrared range. The results of the research are expected to have scientific and practical significance in the creation **of a new generation of** semiconductor devices based on Ge-Sn alloys.

DFT (Density Functional Theory) was used to study the electronic properties of the zone **structure (energy zones) of a solid mixture $Ge_{1-x}Sn_x$** , which is the **most efficient**

quantum mechanical method of our time. DFT is an approximate and simplified version of the Schrödinger equation, not the complete solution of . This method makes it possible to determine their total energy, zone structures, transition zones and other quantum properties by calculating the electron density within a material.

For the computational work, **the Quantum ESPRESSO** software package was chosen. This program is open source and has the ability to perform most DFT-based calculations. With it, interatomic potentials (pseudopotentials), wave functions, and energy spectra were calculated. The Xmgrace program was used to draw graphs. In addition, **the k·p (k point and p operator) model** was used to analyze the obtained results . This model helped to represent realistically calculated zone structure data through mathematical formulas and to understand their behavior with simple models

We first studied the electron zones, total energy, and stability in studying the properties of the Ge_{1-x} Snx semiconductor solid mixing zone. Secondly, for this we performed computer calculations via DFT,thirdly, knowing that in DFT calculations 2 important parameters must be precisely selected, otherwise incorrect results will be obtained

-evutwfc- Wave function shear energy

- k-point (nk1=nk2=nk3) - we have seen how precise the crystal lattice is, and the calculation of the electron at each point.

To investigate the properties of the semiconductor solid mixture zone structure Ge1-x Sn_x to check which computational precision is suitable:

1. The kinetic energy of the flat wave was converged with total energy;
2. With total energy, the k-point values in the Brillouin zone were converged.
3. We determined the optimal lattice parameter of Ge(german).
4. Through DFT calculations of the Ge (germanium) ban zone, we saw that Ge=0.66 eV.
5. Energies were calculated for 300 k points.

1.The kinetic energy of the flat wave was converged with the total energy.

From doing this, it is clear from the theory of purpose that electrons are treated as flat waves, while flat waves are kinetic energy. A wave function corresponds to each electron. This graph shows the kinetic energy of the wave function on the x axis, i.e., the kinetic energy of the cut. We did this to get the optimal option for the later calculations, because as you can see from this graph, the total energy of this system is changing, i.e. at ecutwfc 60, the total energy has not changed, the energy has stabilized, otherwise the calculation will fail to use this value for further calculations. Doing this will definitely save time, and when the energy is stabilized, the calculations will be correct. (Figure 1.1)

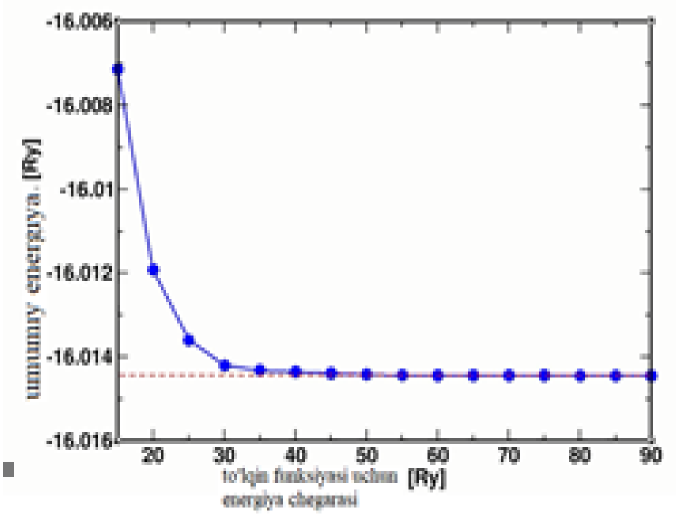


Figure 1.1. Convergence of Kinetic Energy of a Flat Wave with Total Energy

2. With total energy, the point values k in the Brillouin zone were converged and the optimal variant was determined.(Figure 1.2)

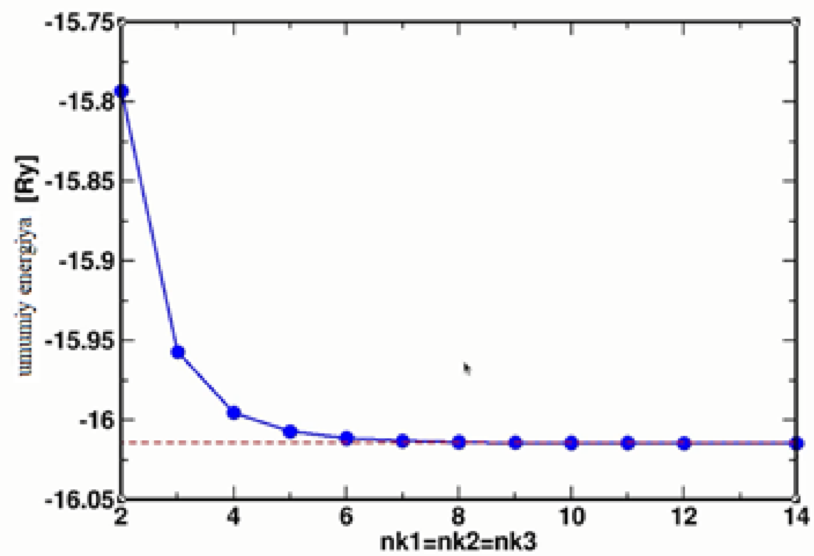


Figure 1.2. Convergence of point values k in the Brillouin zone with total energy

This graph basically shows the k-point result made in our DFT calculations, i.e., it was determined that the Brillouin zone size is 8.

3.Ge (Germanic) determined the optimal lattice constant. The graphic is shown below.(Figure 1.3)

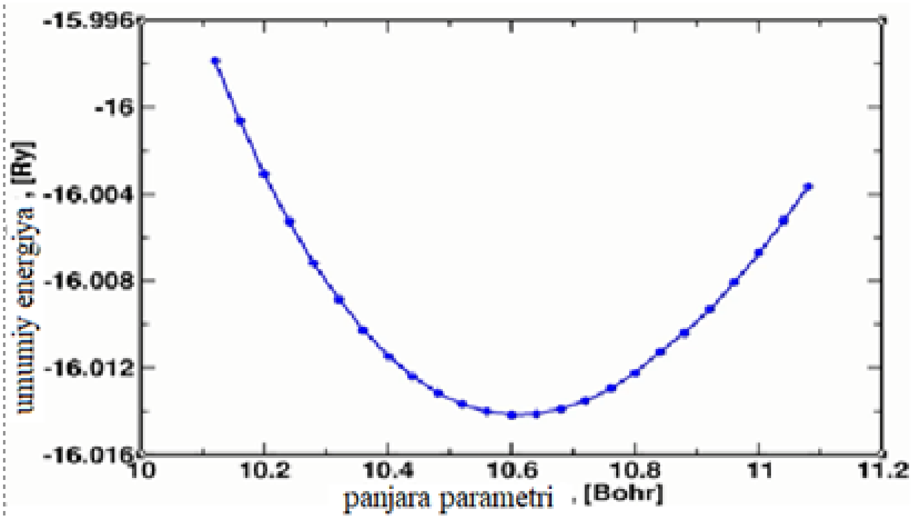


Figure 1.3. Graph of the optimal lattice constant of Ge(german)

The optimal lattice constant of Ge (germanium) was obtained through DFT calculations at 10.6094 units, 5.61427 A^o (angstrem) units. Ge was then computed as follows, knowing that the lattice constant from which Ge was obtained experimentally was 5,657 A^o.
5,657 A0 -5,61427 A^o = 0,04273
0.04273: 5.657=0.007553474
That is, the error came out of 0.0075%, which means that it is almost identical to the expression. For further calculations, we took the lattice constant Ge (germanic) as a unit value of 10.6094 Bor.

4.Ge (German) was considered a no-go zone through the DFT. The graph below was taken. (Figure 1.4)

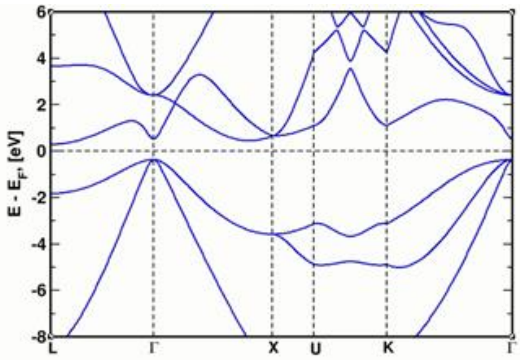


Figure 1.4. This graph shows the structure of the energy zones of germanium (Ge) in the crystalline state**.**

Based on the results of the 3 studies performed above, we calculated that the bandwidth of Ge in DFT calculations is 0.66 eV. In DFT, we calculated at a low temperature of about almost 0K. In this:

valent zone maximum- 5.5795 eV;

The transmission zone was a minimum of -6.2422 eV.

It turned out to be 6.2422-5.5795= 0.66 eV. It's almost homogeneous with Exprimation.

The results we calculated this were carried out for 2 atoms. For many atoms, calculations would take a lot of time.

The graph of the structure of the energy zones in the crystalline state **shows the following.**

Y-axis (E – EF [eV]): This is the energy of the electrons.**Point 0 — EF (Fermi level):** The energy level that separates the unfilled and filled zones.**X-axis:** Directions of symmetry at different points of the crystal:**L, Γ, X, U, K** are special points within the crystal grid (points in the brillouin zone)Important points in this are:

1.Valent zone (bottom lines, bottom)

-These are the highest energy levels where electrons reside.

The Fermi level is below (0 eV).

2.Permeability zone (top lines, above)

-This is where free electrons can move.

3.Forbidden zone(energy range):

-The space between the zones at the top and bottom of the Fermi level.

-Germanium **does not have a direct busy gap** — that is, the maximum valent band and the minimum conductivity zone are not **at the same k-point**. It' **s called an indirect busy**.

Influence of the element Sn on the zone structure of the $Ge_{1-x}Sn_x$ solid: analysis using DFT and k·p models

The study of the electron zone structure of the $Ge_{0.97}Sn_{0.03}$ solid mixture formed by the addition of 3% tin (S) to germanium currently occupies an important place in semiconductor technology. Using DFT (Density Functional Theory) and k·p methods, the zone structure and inter-zone energy variation are determined. This work was made possible through the Quantum ESPRESSO program.

For the calculations, the first principle-based DFT method was chosen. Quantum mechanical calculations were carried out in the Quantum ESPRESSO program. The K·p model was used to identify and analyze the zone structure.

The calculations made on the basis of the DFT were organized as follows:

- **Pseudopotential:** Meta-GGA (r^2SCAN) functionality was used.
- **ecutwfc (cut kinetic energy):** 60 Ry was selected based on the previous convergence graph.

- **K-dot grid (nk1 = nk2 = nk3):** 8 × were selected according to 8 × 8 (based on convergence).
- The German optimal lattice constant is defined as 10.6094 (in Bohr units).
- Germany's no-go zone width was found to be 0.66 eV.
- **Structure Optimization:** Optimized the supergrid configured for $Ge_{0.97}Sn_{0.03}$.
- **Element addition:** 3% of the atoms in the germanium crystal lattice have been replaced by Sn.

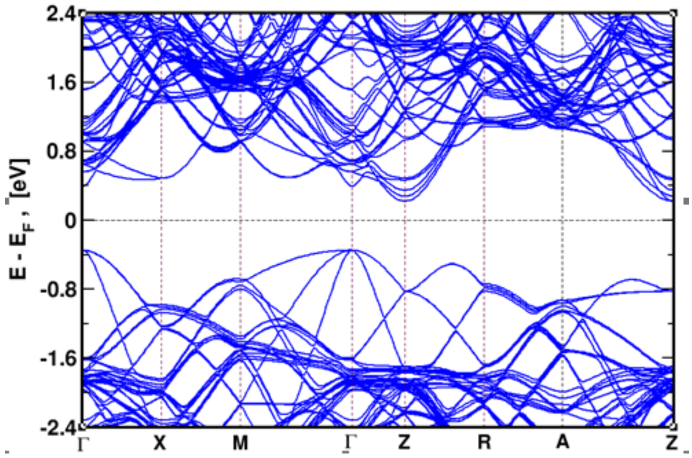


Figure 2.1. $Ge_{0.97}Sn_{0.03}$ Zone structure for solid mix

From the zone structure, it can be seen that under the influence of the Sn mixture, the forbidden zone narrows and the permeability zone shifts downwards (Z –point). The valaent zone shifts upwards (G-spot). That is, the Valent zone maximum for $Ge_{0.97}Sn_{0.03}$ is 5.703 eV

O‘tkazuvchan zona minimum – 6.283 eV

Eg = 6.283-5.703 = 0.56 eV

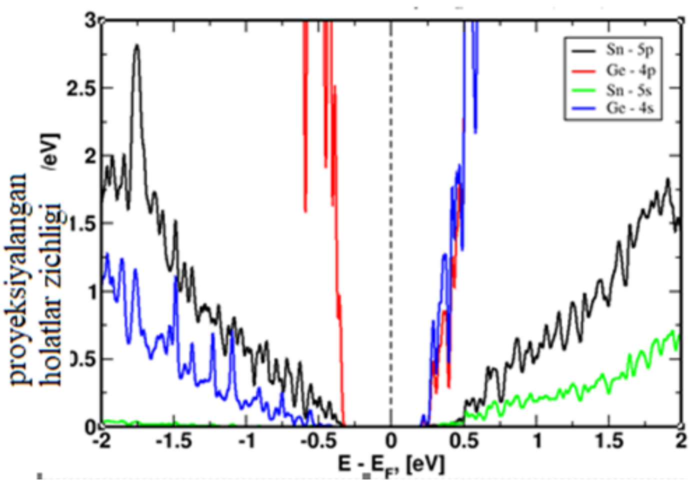
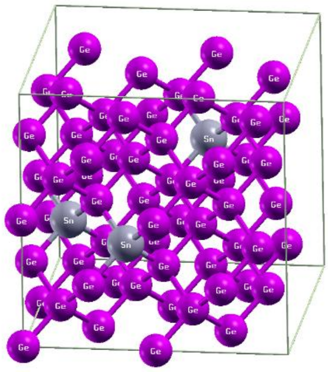


Figure 2.2. The projected state density of $Ge_{0.97}Sn_{0.03}$ solid mixture.

As can be seen from the density state graph, there is a clear gap between the valent zone on the left and the permeability zones on the right, and it shrinks with increasing Sn concentration. As can be seen from the graph, the solid mixture $Ge_{0.97}Sn_{0.03}$ is a semiconductor with a low electron state density near the exclusion zone, the p-orbits of the Ge atom are involved in the formation of the stress zone, and the s-and p-orbits of the Sn atom are involved in the formation of the permeability zone. These results were obtained using the r2scan (Meta-GGA) function using DFT calculations.



2.3-rasm. 2x2x3 Superhujayra

All of the above results were obtained from the same supercell. There are 96 atoms in it. The results indicate that the Sn concentration decreases as the Sn concentration increases, which causes $Ge_{1-x}Sn_x$ mixtures to be of interest in infrasonic and infrared applications.

Sn soni	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	Hajm (Å³)
0							
3	11.2879	11.2879	16.9298	90.002	90.002	90.0015	2157.1226
4							
5							
6							
7							
8							

Figure 2.4. Variation of crystal lattice parameters and size depending on the Sn concentration of the solid mixture $Ge_{1-x}Sn_x$.

The optimal lattice constant of Ge (germanium) was obtained by DFT calculations at 10.6094 bor, 5.61427 A° (angstrem) units. After the addition of 3 % Sn (tin), 5.643 A° became (angstrem), i.e. 10.6643 Bohr.That is, the lattice constant increases regularly with increasing Sn, which is explained by the large radius of Sn atoms in the solid alloy composition. The lattice constant increases regularly with increasing Sn volume, which is explained by the large radius of Sn atoms in the solid mixture structure.

$a_{Ge1-x\,Sn_x}=(1-x)*a_{Ge}+x*a_{Sn}$ (3.3.1)

where: a_{Ge}=10.64 Bohr- the optimal lattice constant for pure Germanic,
aSn = 11.45 Bohr – lattice constant for tin
x=0.03 – Sec concentration (i.e. 3%)
Compute:
$a_{Ge0.97\,Sn0.03}=0.97*10.64+0.03*11.45=10.6643$ Bohr
That is, when 3% Sn is added to Ge, the grid constant is 10.6643 Bohr.
In conclusion, the results of the $Ge_{0.97}Sn_{0.03}$ solid mixture studied using DFT and k·p methods showed:
- As a result of the addition of Sn, the bandwidth (bandwidth) decreases, i.e. it is around 0.56 eV. That is, the straight pass is 0.714 eV, the false pass is 0.56 eV. This means that the valent and conductive zones are approaching due to Sn atoms. The Sn atoms changed the curvature of the zones—which means weaker mass (effective mass) and better conductivity.
- There will be significant changes in the electronic structure. Due to the addition of Sn, it was seen that the maximum energy point in the valent band was slightly elevated and the minimum point in the conduction zone was lowered. These were determined by the k.p model, that is, this model helped validate the results obtained through DFT by a simpler generalized mathematical formula.
- The grid constant increases.
- The novelty of this case is:
The accuracy of the zone structure for $Ge_{0.97}Sn_{0.03}$ has been calculated at a high level.
For the previous Ge, the calculated BFT value (0.66 eV) proved to be reduced to **0.56 eV** after adding Sn. This makes it possible for Ge-based optoelectronic devices **to operate in the low-energy (infrared) ranges**. The computational study of the Ge-S system can be used as a basis for experimental work
These results confirm that $Ge_{1-x}Sn_x$ mixtures are a promising material for optoelectronics and infrared technologies.

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