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Electrical, optical properties and Thermal conductivity of MB_{66} (M- Rare-each elements) boron-rich compounds

TadjievA.A., (Ph.D), Zhabborov A.B.

Assistant Proff, Department of Radio Devices and Systems,Tashkent State Technical University, Tashkent, Uzbekistan
Assistant, Department of Radio Devices and Systems,Tashkent State Technical University, Tashkent, Uzbekistan

ABSTRACT: Investigations of the electrical and optical properties and thermal conductivity of a number of MB_{66} compounds have been carried out (M = Gd, Sm, Yb, Dy, Y). Their properties were compared with the properties of amorphous boron. Amorphous boron and MB_{66} compounds were shown to be materials-analogs due to the specific complex lattice of MB_{66} (amorphization at the atomic scale).

KEYWORDS:Amorphous boron,electrical properties, conduction mechanism, β-rhombohedral boron, fermi level.

I. INTRODUCTION

The electrical and other properties of amorphous boron have been studied in recent years [1-2] during which the hydrogenated amorphous boron films produced by either pyrolysis or glow discharge decomposition of diborane were of interest. These materials seem to be promising for solar cell application [3]. However, there is one more problem which should be developed in the light of recent advances made in amorphous semiconductor physics and applications. This is the so-called "amorphization problem" which has been of interest in particular in connection with microcrystalline films investigations [1]. The conditions of the transition from "crystalline" to "amorphous" properties depending on the material disorder have been under consideration.

It is known that there are a number of ways to change this disorder. This is controlled by grain size [4], concentration of vacancies [5] or spatial fluctuation of composition.Amorphization at an atomic scale can be observed in the case of materials with a complex lattice on the basis of boron [6]. The standard band conduction mechanism is realized for α-rhombohedral boron (12 atoms in the unit cell) in contrast to other materials, boron modifications and compounds - their structural analogs, the unit cells of which contain more than 50 atoms in the unit cells. The specificity of these semiconductors is not only the many atoms in the unit cell but its very complex structure, for instance, several groups of non-equivalent boron atoms with various coordination numbers, various positions of metal atoms in the lattice of the compounds etc[7]. So, the materials on the basis of boron represent a group of semiconductors which are very suitable to develop the "amorphous concept".

A direct comparison of the properties of amorphous boron and β-rhombohedral boron (105 atoms in the unit cell) was made in ref. [2]. Some β-boron properties were shown to be similar to those of amorphous boron: temperature dependence of conductivity and thermoelectric power, but thermal conductivities at low temperatures are quite different for these two materials [2],

The lattice structure of MB_{66} compounds (M- rare earth element) is the most complex among all the boron-based semiconductors (~ 1600 atoms in the unit cell). Thus, these materials must be of interest from the point of view of amorphization at an atomic scale. The purpose of this paper is to consider the properties of MB_{66} in comparison with amorphous boron as it was done earlier for β-boron [2].

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Vol. 3, Issue 12 , December 2016

II. LATTICE STRUCTURE OF MB_{66}

The group of MB_{66} compounds is rather wide (M -Nd, Pm, Sm, Gd, Y, Dy, Ho, Er, Tm, Yb, Lu) [8]. The cubic unit cell contains 1584 boron atoms and 24 metal atoms (the space group is Fm3c).

The main element of the structure is the supericosahedron$B_{12}(B_{12})_{,2}$. These 1248 boron atoms are situated at the summits and at the centers of the cube faces. The lattice constant is equal to 23.44 A. Other boron atoms and metal atoms are situated in the voids. The configurations of MB_{36} and MB_{46} are characteristic of these atoms providing high lattice structure stability. These compounds are known to be very refractory materials [8].

III. EXPERIMENTAL RESULTS

A. Electrical properties and conduction mechanism

The first data on the properties of YB_{66} were obtained in ref. [9]:ρ_{300k}= 360 $\Omega^{-1}cm^{-1}$, $\mu_{300\,K}$< 10 $cm^2\ V^{-1}s^{-1}$, E_g = 1,36eV. The properties of SmB_{66}, GdB_{66}, YbB_{66} (S - thermoelectric power σ - conductivity, R - Hall coefficient) in a wide temperature region were studied in ref. [1]. These data enables us to reach a conclusion that these semiconductors cannot be considered as heavily doped β-rhombohedral boron. This contradicts the conclusion of ref. [2].

Now we shall consider the properties of the materials mentioned and, in addition, of DyB_{66} and YB_{66}. The method of the preparation of DyB_{66} and YB_{66} samples was similar to that which was described in ref. [10]. The electrical parameters of MB_{66} are given in table 1.1.

The properties of amorphous boron used for comparison were taken from refs. [2].

It should be noted that there are the same temperature dependences of the electrical parameters for all MB_{66}. So, these compounds can be considered as the materials-analogs.

The temperature dependences of thermoelectric power(S)and conductivity (σ) of DyB_{66} and amorphous boron are given in figs. 1 and 2. There is the temperature region where S and σ increase simultaneously. Mott's law for conductivity is characteristic of both amorphousboron and MB_{66}, fig. 3a.

Table 1.1Electrical parameters of MB_{66} (S- is the thermoelectric power, σ- the electrical conductivity,E_g- the forbidden gap from σ and S, μ- the Hall mobility, T_0-is from $\sigma \sim \exp[(T_0/T)^{1/4}]$, ΔE is the activation energy, $(\varepsilon_F - \varepsilon_v)_{T=0}$)

S/N	Compound	S, ($\mu V\ K^{-1}$) T= 300 K	σ, ($\Omega^{-1}cm^{-1}$) T= 300 K	E_g,(eV) from σ	E_g,(eV) from S	μ, ($cm^2\ V^{-1}\ s^{-1}$)	T_0 (K)	ΔE (eV)
1	GdB_{66}	+ 390	2×10^{-3}	0,87	0,68	15	$4x10^7$	0,20
2	SmB_{66}	+ 100	10^{-2}	0,80	0,63	15	$2\ x10^7$	0,15
3	YbB_{66}	+ 270	$6\ x10^{-3}$	1,27	1,10	5	$1,2\ x10^6$	0,10
4	DyB_{66}	+ 140	$7,5 \times 10^{-3}$	0,72	0,70	10	-	-
5	YB_{66}	+ 340	$3\ x10^{-3}$	1,00	0,88	10	-	-

The values of thermoelectric power are rather low in this region, fig. 1. Thermoelectric power increases rapidly in the higher temperature region and conductivity increases with a constant activation energy (ΔE), table 1. This is a typical feature of an amorphous semiconductor due to the transitions from variable-range hopping to conduction on the extended states: $\varepsilon_F \rightarrow e_v$ transitions;ε_F - Fermi level, ε_v- mobility edge of the valence band.

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Vol. 3, Issue 12 , December 2016

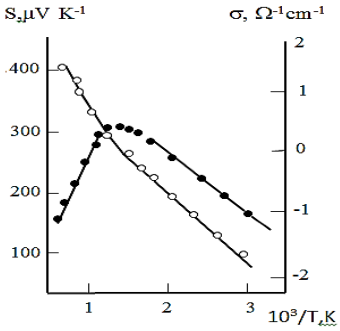


Fig. 3.1.Temperature dependence of (1) thermoelectric power and (2) conductivity of DyB_{66}.

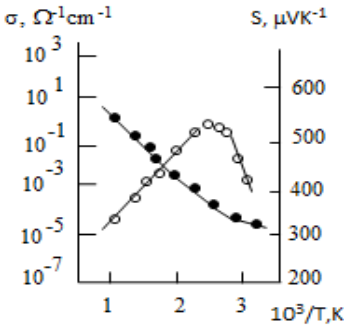


Fig. 3.2.Temperature dependence of (1) thermoelectric power and (2) conductivity of amorphous boron.

Introducing ε_v for MB_{66}, σ can be written as

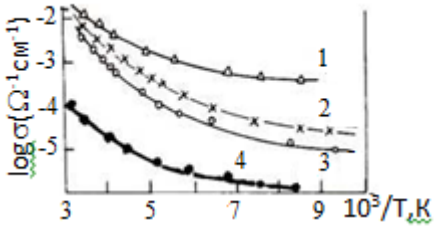
$$\sigma = e\mu_v N_v \exp(\gamma/k)\, \exp(\varepsilon_F - \varepsilon_v)_{T=0}/kT, \qquad (1)$$

where μ_v is the mobility at ε_v, N_v is the effective number of states of the valence band in the kT interval, γ is the temperature coefficient of the $\varepsilon_F - \varepsilon_v$ gap.If a is the experimental value, $N_v \sim 10^{19}$ cm^{-3} and $\gamma = 10^{-4}$eV K^{-1}, μ_v will be of the order of (1-10) cm^2 V^{-1} s^{-1} at T = 300 K. This value is close to the Hall mobility value, table 1. So, conduction on extended states takes place for MB_{66} at room temperature.

The model of density of states (g(ε)) for MB_{66} is proposed to be similar to that of amorphous boron [1]. The Fermi level of amorphous boron was found to be situated at the tail of the density of states ($\varepsilon_v - \varepsilon_F$ = 0,1eV) [1,11]. The density of states diagram of MB_{66} is given in fig. 3b.

The dashed section of the diagram represents the empty states. According to the model the tail for all MB_{66} is the same but the positions of the Fermi level are different. For instance, $T_0 \sim 1/g_{\varepsilon F}$ is lower for GdB_{66} than T_0 for YbB_{66}, table 1.1. Thus, the value of $\varepsilon_v - \varepsilon_F$ for GdB_{66} must be higher. Indeed, it can be seen from table 1. Sm_{66} takes an intermediate position.

a) b)



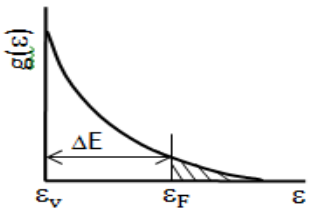


Fig. 3.3.(a) Temperature dependence of the conductivity of (1) YbB_{66}, (2) SmB_{66}, (3) GdB_{66} and (4) amorphous boron in the low temperature region, (b).Density of states diagram of MB_{66}.

ISSN: 2350-0328

International Journal of Advanced Research in Science, Engineering and Technology

Vol. 3, Issue 12 , December 2016

B.Absorption spectra

There are two main features of the absorption spectra both of amorphous boron and MB_{66}. First of all, Urbach's tail is observed, fig.3.4a. Secondly, there are noIR-absorption bands.

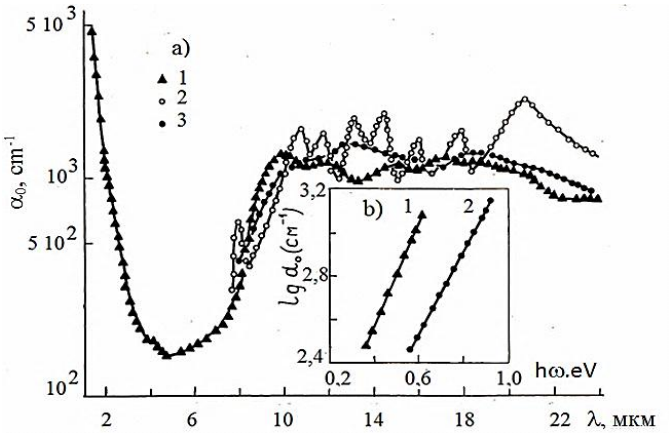


Fig. 3.4. (a) IR-absorption for (1) $GdB_{66}$and (2) amorphous boron, (b)Urbach's tail for (1) GdB_{66} and (2) amorphous boron.

So, the optical properties of β-rhombohedral boron and ofMB_{66}compounds are quite different [1]. Urbach's tail is not observed for β-boron. As for the IR-absorbtion of β-boron a number of very intensive peaks of lattice absorbtion ($\alpha > 10^3$ cm^{-1}) are at $\lambda > 8$ mkm.

C.Thermal conductivity

The thermal conductivity of GdB_{66} depending on temperature is shown in fig. 5. This is typical for all MB_{66} compounds. Thermal conductivity is constant in a wide temperature region as in the case of amorphous boron, fig. 5.

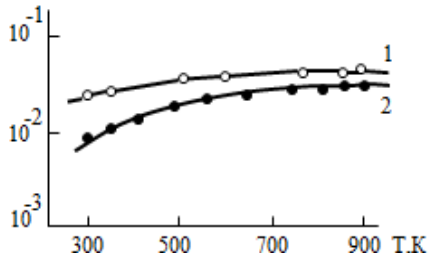


Fig. 3.5.Temperature dependence of the thermal conductivity of (1) GdB_{66} and (2) amorphousboron.

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Vol. 3, Issue 12 , December 2016

It should be noted that the thermal conductivity of β-rhombohedral boron is constant only in the high temperature region. It fails in the low temperature region. The model of thermal conduction for β-rhombohedral boron was proposed in ref. [2]. This model can be applied to other boron-based semiconductors with complex lattices.

IV. CONCLUSION

The consideration of the electrical and optical properties and thermal conductivity of MB_{66} compounds shows they are the materials-analogs. Their properties are like those of amorphous boron.

The density of states model proposed is based on the following experimental facts:

- variable-range hopping,
- correlation between T_0 and ΔE values,
- temperature dependences of thermoelectric power and conductivity which are typical for transition from variable-range hopping to conduction on extended states,
- the same order of value of mobility (μ_v) obtained in two independent ways; from formulae (1) and on the basis of conductivity and Hall coefficient measurements,
- Urbach's tail which is known to be due to structural disorder.

This model of the density of states is typical of an amorphous semiconductor, in particular, of amorphous boron. So, the amorphization of the electron spectrum takes place. Besides, the amorphization of the phonon spectrum also takes place. First of all, there are no peaks in the IR-absorbtion of MB_{66} in contrast to β-rhombohedral boron and other boron-based semiconductors with simples lattices. Then, the temperature dependences of the thermal conductivity of MB_{66} and amorphous boron are similar. Both features enable us to reach the conclusion that the properties of MB_{66} compounds are completely analogous to the properties of amorphous semiconductors. Such amorphization is the amorphization at the atomic scale mentioned above.

MB_{66} compounds represent a group of semiconductors which seem to be unique materials. On the one hand, they are refractory semiconductors but on the other they have the properties of amorphous solids.

In conclusion it should be noted that the amorphization at the atomic scale takes place when the size of a unit cell is about 20 A^0. The same grain size is typical in the transition from "amorphous" to "crystalline" properties of silicon films as recently been shown [1]. Although the nature of disorder is quite different in these two cases long-range order seems to have no influence under the same size conditions.

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AUTHOR'S BIOGRAPHY

TadjievAbdukaumAbdulhaevich - Doctor of Philosophy, Assistant Proff. the Department "Radio Devices and Systems"of theTashkent State Technical University named after Beruni. Author of more than 60 scientific publications, including 2 patents.

ZhabborovAlibekBotirkulugli–Assistant of the Department « Radio Devices and Systems» of the Tashkent State Technical University named after Beruni. Author of more than 9 scientific articles in scientific and technical journals and publication