

STUDY OF STOICHIOMETRICAL COMPOSITION IN OBTAINING TERTIARY COMPOUNDS

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Abstract: This article studies the calculation of stoichiometric composition in the preparation of ternary alloys, n-type and p-type semiconductor thermoelectric alloys.

Keywords: tertiary alloy, tellurium, bismuth, thermoelectric material, quartz crucible, stoichiometric composition, alloy, antimony

Introduction

In recent years, as a result of the extensive development of science and technology, the demand for semiconductor materials opens up a wide range of work to be done in the future of electricity supply in terms of the technologies of the electric power industry. Based on them, they are widely used in semiconductor devices, energy converter devices, thermobatteries of autonomous current sources, and computer equipment. If all these technologies of obtaining thermoelectric materials are implemented in different ways, the characteristics of the materials obtained by these methods will also be different.

Accordingly, the methods of obtaining thermoelectric material have their own advantages and disadvantages. Therefore, we will consider the production of Bi₂Te₃-Sb₂Te₃ thermoelectric material under inert gas pressure. It is known that the alloying substances are developed in different factories, and their level of purity is also different. Alloys obtained from such materials sometimes do not provide the required level of characteristics. In order to obtain a base suitable for alloying from the substances included in the alloy, adding additional chalcogenides to the characteristic $\alpha=200-240$ $\sigma=400-600$ $\text{Om}^{-1} \cdot \text{sm}^{-1}$ and Bi, Te, Se, Sb included in its triple composition materials are selected, that is, the stoichiometric composition of Bi₂Te₃ – Bi₂Se₃ and Bi₂Te₃ – Sb₂Te₃ base is theoretically found for the following p and n type materials.

Accordingly, for n-type Bi₂Te₃ – Bi₂Se₃ composition

Bi-54.1678 mol %, Te-39, 6924 weight %, Se-6.1398 mol %,

For p-type Bi₂Te₃ – Sb₂Te₃ composition, Bi-16,179 mol %, Te-56,993 mol %, Sb-26,828 mol % are found. For example, for n-type Bi₂Te₃ - Bi₂Se₃ thermoelectric materials, the following calculations are carried out by accurately weighing the above-mentioned substances on a scale.

Calculation of the stoichiometry of binary alloys

Bi₂Te₃

Atomic weight of bismuth, Bi-208,980

Atomic weight of tellurium, Te-127.60

Bi₂Te₃ can be written 2Bi+3Te then

$2 \cdot 208,980 + 3 \cdot 127,60 = 417,96 + 382,8 = 800,76$

We determine the amount of bismuth and tellurium by proportion

800,76 — 100%



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$$417,96 \text{ — } X_{\text{Bi}}$$

$$X_{\text{Bi}} = \frac{417,96 \cdot 100}{800,76} = 52,195 \approx 52,2$$

$$800,76 \text{ — } 100\%$$

$$382,8 \text{ — } X_{\text{Te}}$$

$$X_{\text{Te}} = \frac{382,8 \cdot 100}{800,76} = 47,8$$

To dissolve the stoichiometric composition of Bi_2Te_3

$$\text{Bi} \text{ — } 52,2\%$$

$$\text{Te} \text{ — } 47,8\%$$

It should be taken in grams.

Sb_2Te_3 is calculated in the same way.

2. To calculate the ternary Bi_2Te_3 - Sb_2Te_3 , it is necessary to know the percentage of Bi_2Te_3 and Sb_2Te_3 .

$$\text{If } \text{Bi}_2\text{Te}_3 \text{ - } 26 \%$$

$$\text{Sb}_2\text{Te}_3 \text{ - } 74 \%$$

$$800,76 + 626,3 = 1427,06$$

It is necessary to calculate how many percent of the total atomic weight are Bi_2Te_3 and Sb_2Te_3 .

$$1427,06 \text{ — } 100 \%$$

$$x_{\text{Bi}_2\text{Te}_3} \text{ — } 26\%$$

$$X_{\text{Bi}_2\text{Te}_3} = \frac{1427,06 \cdot 26}{100} = 371,03$$

$$1427,06 \text{ — } 100 \%$$

$$x_{\text{Sb}_2\text{Te}_3} \text{ — } 74\%$$

$$X_{\text{Sb}_2\text{Te}_3} = \frac{1427,06 \cdot 74}{100} = 1056,02$$

To find what percentage of Bi_2Te_3 is Bi or Te

$$371,03 \text{ — } 100\%$$

$$X_{\text{Bi}} \text{ — } 52,2\%$$

$$X_{\text{Bi}} = \frac{371,03 \cdot 57,2}{100} = \frac{19368,76}{100} = 193,67$$

$$X_{\text{Te}_1} = 371,03 - 193,67 = 177,36$$

In the same way, Sb_2Te_3 percentage of Sb or Te is determined.

Let's make a proportion to find what percentage of the total atomic weight is made up of tellurium.

$$1427,06 \text{ — } 100\%$$

$$823,65 \text{ — } x_{\text{Te}}$$

$$X_{\text{Te}} = \frac{823,65 \cdot 100}{1427,06} = 57,71$$

To find antimony



1427,06 — 100%

409,73 — x_{Sb}

$$X_{Sb} = \frac{409,73 \cdot 100}{1427,06} = 28,71$$

To determine Bi

$$X_{Bi} = 100 - 57,71 - 28,71 = 13,58$$

So, to obtain an alloy with a stoichiometric composition of triturated Bi_2Te_3 -26%, Sb_2Te_3 -74%, it is necessary to weigh the following substances by weight.

Sb-28,71g

Te-57,71g

Bi-13,58g

100,0

In practice, the content of the extracted material is loaded into the quartz crucible from top to bottom based on the Bi-Te-Se or Bi-Te-Sb scheme.

As a result, elements with a stoichiometric composition are introduced into the alloy extraction device under the pressure of inert gas.

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