# Determination of Partial Coordinate Number of Atoms in Amorphous Yb-As-S(Se, Te) Systems

**Rasim ALİ-ZADE AHMED OĞLU, Eldar EFENDİYEV HUSEİN OĞLU**
**Elman HAJİYEV SHAMKHAL OĞLU**
*Institute of Physics Azerbaijan Academy of Sciences,*
*Azerbaijan Republic, Baku 370143, H. Javid st. 33*

## Abstract

Partial coordinate number for amorphous compounds, consisting three type of atoms has been determined by way of calculation of the radial distribution curve maximum. The equation solution method has been used as algorithm in programme, which writed in FORTRAN language for working in IBM compatible computers. The programme is compact and integable. The programme has been used for determination partial coordinate number of ytterbium atom in amorphous compounds-$YbAs_2S_4$, $Yb_3As_4S_9$, $YbAs_4Te_7$, $Yb_3As_4Se_9$ $YbAs_4Se_7$. Real value of partial coordinate number of ytterbium in this compunds is 2 or 3.

## 1. Introduction

At present, various approaches exist to describe structureof amorphous compounds (unsystematic net of atoms, crystallite hypothesis, cluster describtion) [1], however for creation single theory of structure of amorphous state it is necessary to obtaine a large number of structural data. Partial coordinate number of atoms and interatomic distance are main structural parameters of amorphous compounds.

Structural peculiarities of amorphous materials are described by correlation function, in particular, binar radial distribution function of atoms density allowed to obtaine structural parameters of amorphous compounds. Electron and X-rays difraction methods, allowing to get radial distribution function W(r) in investigation of the structure of amorphous materials, lead to an integral analysis of experimental curves of intensity. In this case one do not required prelaminary properties about structure, it's enough to get curves of electron scattering or X-rays intensity [3,4].

The areas under the radial distribution maximums as derived from electronographic curves maximums for amorphous materials is related to the concentration of atoms, scat-

tering ability, etc. This correlation for materials having three types of atoms is given by

$$Q_1 = \sum_{i=1}^{3} \sum_{j=1}^{3} C_i K_i K_j n_{ij} \qquad (1)$$

where, n is the number of "j" type of atoms near one "i" atom, $C_i$ is the relative number of "i" type of atoms, K is the scattering ability of "i" type of atoms, Q is the area under the first maximum on the atoms radial distribution function W(r) [5].

Partial coordinate numbers of atoms in amorphous compounds may be determined from formula (1). The employement gradient, tangential, linearisaton and other optmization methods, which required to calculate first and second derivation of the minimization function lead to receiving no whole values of partial coordinate numbers, which in later is necessary to round to whole value [3,4,6]. Moreover, this would require to carry out a lot of work and to spend additional machine time, which lead to errors. Determination of the partial coordinate numbers of atoms in amorphous compounds, containing more than two class of amorphous materials for which there is necessary to know the partial coordinate numbers are the new Yb-As-S(Se,Te) compounds containing rare earth elements (REE) [7]. These types of materials have potential use, containing magnetic f-elements (REE) [7-9]. Also, there is data suggested it may also be used in acousto-optics [10]. The main interest in these materials is the environment of the reare earth atom becouse it determines the electrical, optical and magnetic properties of these materials [1,7].

## 2. Method of determination partial coordinate numbers

We used the coordinate lowering method together the selection method for determination of the partial coordinate numbers of atoms [11]. This method gives rapid and reliable results. Direct summarisation in this method allowed to give whole number of partial coordinate numbers, which are clouse to the real valie. Unlike to above emphasized methods, at using suggested method, there are require to calculate the values of function and to carry out their comparision.

The area under first maximum ($Q_{calc.}$) of the radial distribution curves for a given compound as calculated by Eqn.(1), according to coordinate lowering method and is compared with the experimentally determined value of this area ($Q_{exp}$). If the difference ($Q_{calc.} - Q_{exp}$) is smaller or is equal to given value ($X_{min}$), then fixed value the partial coordinate numbers being in summing up. Thus an algorithm to determine the partial coordinate numbers in amorphous compounds has been devised based on the numerical solution of Eqn. (1). The algorithm has been realised as a compact computer program in FORTRAN on an IBM PC/AT-386 computer system.

## 3. Results and Conclusion

We obtained a set of partial coordinate numbers for each investigated amorphous compounds with using this programme. We made preferable choice of one set of partial

numbers for each of above mentioned amorphous compounds by analysing an interatomic distance and structure data of these compounds in crystal state and used other data obtained before [12-17]. We used this programme for determination partial coordinate numbers for many triple amorphous compounds, in particular for $YbAs_2S_4$, $Yb_3As_4S_9$, $YbAs_4Te_7$, $Yb_3As_4Se_9$, $YbAs_4Se_7$ and it was shown that in these compounds coordinate number for ytterbium are 2 or 3 and the neighbouring atoms of ytterbium are chalcogen atoms. The results obtaining with this programme for these compounds are adduced and analysed in [12-17].

Structure of crystallic compounds $Eu_3Sb_4Se_9$ in bulk state investigated in [17, 18]. It was shown that minimal coordinate number of Eu is equal to 6. Our data showed, that trigonal prism with REE in centre, which is observed for $Eu_3Sb_4Se_9$ and other crystallic ternary compounds with REE, in films amorphous structures is undergoed to distortion in results, which atom (ion) yetterbium is displaced to near three atoms of sulphur. Thus evidently described that, environment of REE, in this case Yb, obtained for coordinate numbers are 2 or 3, moreover all the nearest neighboroughs of Yb atom are chalcogenide atoms.

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