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# Phase diagram of Ge:(C, Sn)

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ABSTRACT

We present the self-assembling conditions of 1C4Sn tetrahedral nanoclusters with carbon atoms in their centers in Ge:(C, Sn) in the wide temperature range as a function of the impurity contents and temperature. These conditions are the phase diagram of Ge:(C, Sn) since nanocluster occurrence and completion of self-assembling when all carbon atoms are in nanoclusters are results of the continuous phase transitions. The significant decrease of the strain energy after formation of nanoclusters is a cause of self-assembling. It is shown that the nanocluster occurrence temperature depends only on the Sn content. The impurity content conditions when all carbon atoms are in 1C4Sn nanoclusters are obtained for the temperatures up to 855 °C.



## 1. Introduction

Single photon devices are crucial elements of quantum computers [1]. Recently, as a material for single photon sources, considerable interest has been renewed in the luminescent properties of semiconductors doped with the isoelectronic impurities forming excitonic traps [2]. The bound excitons form because of the difference in the electronegativities of isoelectronic impurity and host atoms [3]. This difference for carbon and Ge is more than three times larger than that for Bi and phosphorus. However, the data on excitonic traps in Ge:C are absent in contrast to GaP:Bi where isolated impurities form excitonic traps. It can be a result of the lattice strains in Ge:C. The lattice strains around impurities decrease the binding energy and, therefore, play a negative role at the excitonic trap formation [3]. The significant decrease of the lattice strains around carbon atoms can be

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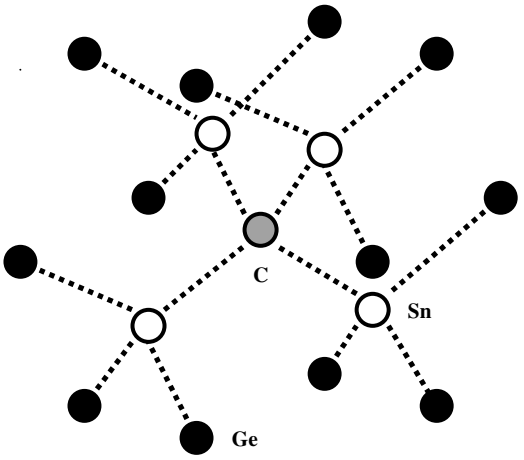


**Fig. 1.** 1C4Sn nanocluster in Ge-rich $C_xSn_yGe_{1-x-y}$ alloy.

reached in Ge:(C, Sn) after self-assembling (SA) of 1C4Sn tetrahedral nanoclusters with carbon atoms in their centers [4]. Therefore, the formation of excitonic traps in Ge:(C, Sn) with 1C4Sn nanoclusters seems highly probable and, thus, Ge:(C, Sn) is a promising material for fabrication of single photon devices. The equality conditions of the free energies of random alloys and alloys in which all carbon atoms are in 1C4Sn nanoclusters were obtained [4]. However, the SA conditions of 1C4Sn nanoclusters are not developed yet.

The SA conditions of 1As4Ga nanoclusters in zinc blende AlN:(Ga, As) were obtained in [5] by a phase diagram since an occurrence of nanoclusters and completion of SA when all As atoms are in nanoclusters should be the results of the continuous phase transitions. The phase diagram describes a fraction of As atoms situated in nanoclusters as a function of the impurity contents and temperature. Later, similar diagrams were also obtained for the other semiconductors with the zinc blende structure [6]. However, the strain energies and configurational entropies of the doped semiconductors with the zinc blende and diamond structures should be different. Therefore, the approach from [5] cannot be extended to Ge:(C, Sn). The aim of this paper is a consideration of the SA conditions of 1C4Sn nanoclusters in Ge:(C, Sn).

## 2. Model

Double doping with carbon and Sn transforms Ge into Ge-rich $C_xSn_yGe_{1-x-y}$ substitutional alloy with the tetrahedrally coordinated impurities. Redistribution of atoms in $C_xSn_yGe_{1-x-y}$ does not change its chemical composition. Therefore, only the free energy of mixing depending on the atomic arrangement is taken into account. The free energy of mixing of $C_xSn_yGe_{1-x-y}$ is represented as a sum of the strain energy and configurational entropy term $f^M = u^{SE} - Ts^C$. Carbon in the ultra-dilute limit and the Sn content $y > 4x$ are considered. The strain energy is given as

$$u^{SE} = \alpha x u_{1C4Sn} + (1-\alpha)x u_C + (y - 4\alpha x)u_{Sn} \tag{1}$$

where $\alpha$ is a fraction of carbon atoms situated in nanoclusters and $u_{1C4Sn}$, $u_C$ and $u_{Sn}$ are the strain energies caused by 1C4Sn nanoclusters shown in Fig. 1, by isolated carbon and by isolated Sn atoms, respectively.

The strain energies caused by nanoclusters and by isolated impurities were represented as sums of two items. The first item is the deformation energy of quadruple of tetrahedral cells situated around carbon atoms in 1C4Sn nanoclusters or around isolated carbon or around isolated Sn atoms. These energies were described using the valence force field model [7]. The averages of the bond stretching and bond bending elastic constants were used as the bond stretching and bond bending