Study of structural properties of alloy Tl\textsubscript{x}Ga\textsubscript{1-x}N

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Abstract. The structural properties of Tl\textsubscript{x}Ga\textsubscript{1-x}N have been examined by the use of interaction potential model (IPM). Interaction potential model (IPM) is made up of Coulomb interaction, three-body interaction, van der Waal interaction and short range overlap repulsive interactions. The structural properties namely phase transition, volume collapse for the present alloy have been computed via vegard’s law. We have also investigated the elastic properties i.e. second order elastic constants, bulk modulus, shear modulus, Pugh ratio and anisotropy factor. These elastic properties are the first attempt for the present alloy.

1. Introduction

The combination of III group and V group reveal the new III-V alloys. These alloys are more suitable for the purpose of electronic and optoelectronic devices. Various III-V semiconductor alloys have been studied but there is no experimental study available for the synthesis of alloy of thallium containing nitride. Also the theoretical reports are very less on them. The Tl\textsubscript{x}Ga\textsubscript{1-x}N is regarded as wide band gap semiconductors ranging from ultraviolet to visible regions of the spectrum. It has a very high thermal conductivity and large bulk modulus and makes them important material [1]. Thallium containing nitride bears the advantage more than II-VI compounds due to which they are good alternates to II-VI compounds. Houat et al. [1] have offered the structural and optical properties of alloy Tl\textsubscript{x}Ga\textsubscript{1-x}N through first-principle calculations. To expand the structural and elastic properties we present the systematic and comparative study. In order to depict the present alloy we employ the theoretical approach viz interaction potential model (IPM) in the present study. We applied this IPM to study the phase transition, volume collapse and elastic properties of Tl\textsubscript{x}Ga\textsubscript{1-x}N. In the present model we have incorporated the Coulomb interaction, three-body interaction (TBI), van der Waal (vdW) interaction and short range overlap repulsive interaction. All the properties have been calculated by using Vegard’s law.

2. The potential model and method of computation

The chief part of our theoretical method (IPM) is TBI. To understand TBI we first define the many body interaction (MBI). We know that as the pressure is applied on crystal then its volume decrease owing to this there is exchange of charges between the overlapping electron shells of the adjacent ions. This overlapping provides the transfer of charges and these charges interact with other charges which are present in the cumblic field. This mechanism is called many body interactions (MBI), the important part of MBI is three-body interactions TBI [2].

The Gibbs free energy (G=U+PV-TS) has included the TBI effects. Noted that, U is the lattice energy, P is pressure, V is volume and S is the entropy at absolute temperature T. At zero temperature and pressure, the Gibbs free energy for the zinc-blend (B3) and NaCl (B1) structures are
\[ G_x(r) = U_x(r) + PV_x \]  
\[ G_y(r) = U_y(r') + PV_y \]  

Here X and Y stands for B3 and B1 phase. The primary terms \( U_x(r) \) and \( U_y(r') \) are the lattice energy and secondary are pressure-volume term of both phases. We have added several interactions in lattice energies to develop IPM.

\[ U_x(r) = U_x(Col) + U_x(TBI) + U_x(vdW) + U_x(OR) \]  
\[ U_y(r') = U_y(Col) + U_y(TBI) + U_y(vdW) + U_y(OR) \]

Where former is lattice energy of coulomb interaction, next is lattice energy of TBI, after that lattice energy of van der Waal interaction and last is overlap repulsive energy.

3. Results and discussions

For studying the problems of alloy of III-V semiconductors we generally take the Vegard’s law [3] which states that the atoms are located at the ideal sites and the lattice constants vary linearly with composition x.

\[ a(A_x B_{1-x} C) = xa_{AC} + (1-x)a_{BC} \]  

here AC and BC stands for TlN and GaN, x is concentration and “a” is lattice parameter for pure mixed compound.

First we have calculated the model parameters, following method given in our previous work [4]. By the use of Vegard’s law and model parameters we have computed the structural properties viz phase transition pressure and volume collapse for present alloy Tl\(_x\)Ga\(_{1-x}\)N. Fig.1 (a-b) shows the variation of phase transition pressure and volume collapse with concentrations. It is obvious from this figure that as the concentrations increases the phase transition pressure and volume collapse decreases.

![Figure 1(a-b)](image)

**Figure 1(a-b).** Variation of phase transition pressure and volume collapse with concentration.

Next we have studied the elastic behavior with concentrations of this alloy to enhance the applicability of our model. To get this we have determined the second order elastic constants (C\(_{11}\), C\(_{12}\), C\(_{44}\)) for the pure compounds after this through the Vegard’s law we obtained the second order elastic constants for mixed compound i.e. Tl\(_x\)Ga\(_{1-x}\)N at different composition x. The method for calculations of second order elastic constants is same which we have reported in our earlier work [4]. The calculated values of C\(_{11}\), C\(_{12}\) and C\(_{44}\) are listed in Table 1 and they are compared with available theoretical results for pure compounds.
Table 1. Elastic constants - bulk and shear modulus of Tl_xGa_{1-x}N.

| Compounds      | C_{11} (GPa) | C_{12}(GPa) | C_{44}(GPa) | B(GPa)  | G (GPa)  |
|----------------|-------------|-------------|-------------|---------|---------|
| GaN            | 278.96      | 177.0       | 186.97      | 210.98  | 66.31   |
| Tl_{0.25}Ga_{0.75}N | 251.63      | 163.26      | 160.85      | 192.05  | 57.12   |
| Tl_{0.5}Ga_{0.5}N | 224.30      | 149.53      | 134.73      | 174.45  | 47.94   |
| Tl_{0.75}Ga_{0.25}N | 196.97      | 135.80      | 108.61      | 155.19  | 38.75   |
| TIN            | 169.65      | 122.07      | 82.5        | 137.93  | 29.56   |
|                | 194.3[6]    | 114.5[6]    | 103.2[6]    | -       |         |

The variation of second order elastic constants (SOECs) with pressure at different concentrations (x) is shown in figure 2. It is clear from this figure as the pressure increased the SOECs also increased at different concentrations (x=0, 0.25, 0.5, 0.75, 1.0). This influence is more pronounced in C_{11} as compared to C_{12} and C_{44}.

![Figure 2](image_url)

Figure 2. Variation of C_{11}, C_{12}, C_{44} with pressure at different concentrations X.

The variation of bulk modulus and shear modulus at different concentrations are shown in table 1. It is noticed from this Table that as the concentrations of TIN increased the bulk modulus and shear modulus decreased. No compression could be made due to unavailability of experimental and theoretical results.

To identify the ductile and brittle nature of materials there are various way to obtain this. For the sake of simplicity we computed the pugh ratio B/G. It has a decisive value for separating the brittle and ductile nature i.e. 1.75. Ductile material having the value equal or above 1.75 while brittle
material possess the value below 1.75. Looking the Fig. 3 we can say that our studies represent the highly ductile nature of mixed compound and this behaviour enhance with concentrations.

Since the anisotropic factor A is a property related to the micro cracks in the materials and one important feature of this is measurement of isotropic and anisotropic nature of materials. It is one for isotropic and greater than one for anisotropic materials. Fig.3 shows the anisotropic behaviour of present alloy with concentrations.

![Figure 3. Variation of Pugh ratio and anisotropy factor with concentrations X.](image)

4. Conclusions
The structural properties like phase transition and volume collapse of alloy Tl,ZrGa1-xN are analysed. The pressure dependence of SOECs will provide valuable information on the valuable quality of the solids. The Bulk (B) modulus, Shear modulus (G), Pugh ratio (B/G) and anisotropic factor for the present mixed compound are analysed for the first time. Ultimately it may be concluded that, the IPM approach is sufficiently suitable for structural and elastic properties of Tl,Ga1-xAs alloy. Our results may be tested with different theoretical and experimental workers.

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