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Poisson Ratio and Biaxial Relaxation Coefficient in $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ Alloys

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We present theoretical results showing dependence of Poisson ratio and biaxial relaxation coefficient on composition and atomic arrangement in wurtzite $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys. Our calculations reveal that the Poisson ratio determined for $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys subjected to a uniaxial stress parallel to the c axis of the wurtzite structure shows significant superlinear dependence on composition. The superlinear bowing in Poisson ratio is enlarged by the effect of In clustering. The biaxial relaxation coefficient determined for $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys subjected to a biaxial stress in the plane perpendicular to the c axis of the wurtzite structure changes superlinearly and linearly with x in $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$, respectively. The effect of In atom clustering results in sublinear dependence of the biaxial relaxation coefficient in both $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys.

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1. Introduction

Wurtzite $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys are strategic materials for use in light emitting devices. Although remarkable progress has been made in development of GaN-based optical electronic devices in recent years, many fundamental properties of group III nitride alloys and quantum structures are not yet sufficiently well understood. In particular, the influence of strain and In fluctuations on the electronic band structure of nitride alloys and quantum structures are still the subject of vigorous debate [1–4]. Our recent *ab initio* study of the elastic constants in $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys has revealed that the commonly used Vegard-like rule, i.e., linear dependence on the alloy content, can be accepted only for selected elastic constants [5]. We have also shown that the effect of clustering of In atoms in $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ influences significantly the elastic constants whereas it changes little the bulk modulus [5].

In the present work, we investigate Poisson ratio, ν_c, in $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys subjected to a uniaxial stress parallel to the c axis of the wurtzite structure, and biaxial relaxation coefficient, R_c, determined for these alloys subjected to biaxial stress in the plane perpendicular to the c axis. Particularly, we show that contrary to the bulk modulus, the influence of In clustering is significant for the composition dependence of both ν_c and R_c parameters.

2. Elastic constants

Performing self-consistent *ab initio* calculations in the framework of the density-functional theory [5], we have found the following composition dependence of the elastic constants in wurtzite $In_xGa_{1-x}N$ (1a)–(1e) and $In_xAl_{1-x}N$ (2a)–(2e) alloys (in GPa):

$$C_{11} = 368(1-x) + 229x - b_{11}x(1-x)\,, \tag{1a}$$

$$C_{12} = 153(1-x) + 116x - b_{12}x(1-x)\,, \tag{1b}$$

$$C_{13} = 117(1-x) + 97x - b_{13}x(1-x)\,, \tag{1c}$$

$$C_{33} = 400(1-x) + 238x - b_{33}x(1-x)\,, \tag{1d}$$

$$C_{44} = 92(1-x) + 50x - b_{44}x(1-x)\,, \tag{1e}$$

$$C_{11} = 397(1-x) + 229x - b_{11}x(1-x)\,, \tag{2a}$$

$$C_{12} = 145(1-x) + 116x - b_{12}x(1-x)\,, \tag{2b}$$

$$C_{13} = 115(1-x) + 97x - b_{13}x(1-x)\,, \tag{2c}$$

$$C_{33} = 371(1-x) + 238x - b_{33}x(1-x)\,, \tag{2d}$$

$$C_{44} = 115(1-x) + 50x - b_{44}x(1-x)\,, \tag{2e}$$

where the bowing parameters, b_{ij}, take the values $b_{11} = 60(100)$, $b_{12} = 14(43)$, $b_{13} = -4(-4.5)$, $b_{33} = 71(-1)$, $b_{44} = 16(35)$ for $In_xGa_{1-x}N$, and $b_{11} = 80(141)$, $b_{12} = 8.7(47)$, $b_{13} = -3(-11)$, $b_{33} = 25(-93)$, $b_{44} = 35(70)$ for $In_xAl_{1-x}N$. The values of b_{ij} not contained in brackets were found for alloys with uniform distribution of In atoms (uniform alloys) whereas the numbers in brackets correspond to b_{ij} in the alloys with clustered In atoms on cation sites (clustered alloys) [5].

3. Poisson ratio

The Poisson ratio for wurtzite materials compressed or stretched along the c axis (z-direction) determines the relationship between in-plane strain, ε_{xx}, and strain parallel to the c axis, ε_{zz}, and can be expressed by the elastic constants using the following formula [6]:

$$\nu_c = \frac{C_{13}}{C_{11} + C_{12}} \,. \tag{3}$$

Knowledge of ν_c is very important for determination of alloy film composition and thickness using high-resolution X-ray diffraction measurements [7]. In Fig. 1a and b, we show dependence of ν_c on composition in uniform (solid lines) and clustered (dashed lines) $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}$ and $\mathrm{In}_x\mathrm{Al}_{1-x}\mathrm{N}$ alloys obtained using Eqs. (1)–(3). In these figures, we have also included the curves (dotted lines) showing dependence of ν_c on composition when the Vegard-like rule for C_{ij} (i.e., $b_{ij} = 0$) is assumed. One can see that in $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}$ and $\mathrm{In}_x\mathrm{Al}_{1-x}\mathrm{N}$, for both uniform and clustered alloys, ν_c depends superlinearly on composition whereas sublinear dependence occurs when the Vegard-like rule for C_{ij} is taken into account. The bowing of ν_c is significantly larger for clustered alloys than for uniform alloys that indicates considerable influence of In clustering on the values of ν_c in both $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}$ and $\mathrm{In}_x\mathrm{Al}_{1-x}\mathrm{N}$ alloys.

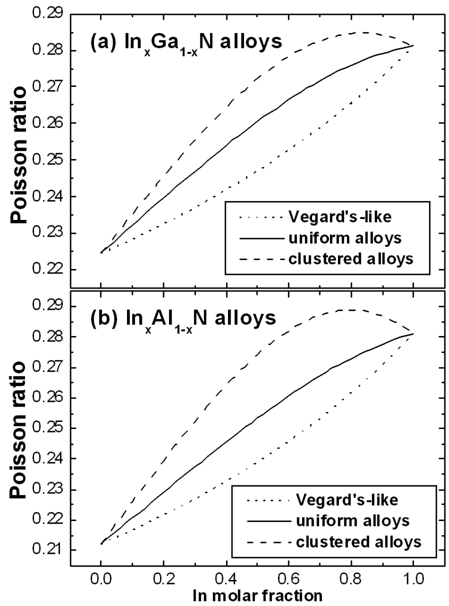

Fig. 1. The composition dependence of Poisson ratio in $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}$ (a) and $\mathrm{In}_x\mathrm{Al}_{1-x}\mathrm{N}$ (b) alloys. Solid and dashed lines are used to show the results obtained for uniform and clustered alloys whereas dotted lines represent the case when the Vegard-like rule for the elastic constants is taken into account.

4. Biaxial relaxation coefficient

The biaxial relaxation coefficient in wurtzite materials subjected to a biaxial stress in the plane perpendicular to c axis determines the relationship between ε_{zz} and ε_{xx}, and can be found using the following expression [6]:

$$R_c = \frac{2C_{13}}{C_{33}} \,. \tag{4}$$

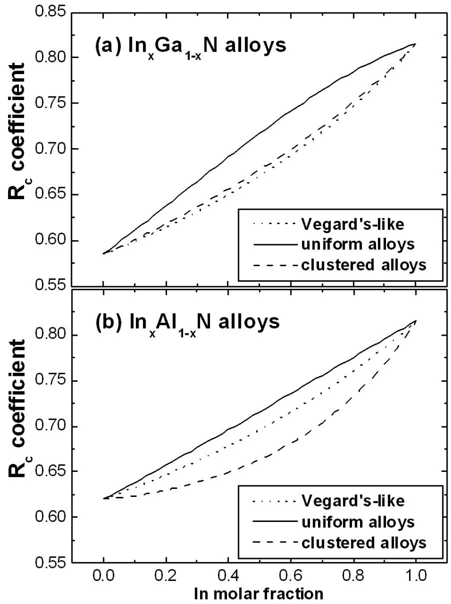

Fig. 2. The composition dependence of the biaxial relaxation coefficient in $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}$ (a) and $\mathrm{In}_x\mathrm{Al}_{1-x}\mathrm{N}$ (b) alloys. Solid and dashed lines are used to show the results for uniform and clustered alloys whereas dotted lines represent the case when the Vegard-like rule for the elastic constants is taken into account.

Knowledge of R_c is crucial for determination of strain in planar heterostructures and quantum structures grown along c axis [6]. In Fig. 2a and b, we show dependence of R_c on composition in uniform (solid lines) and clustered (dashed lines) $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}$ and $\mathrm{In}_x\mathrm{Al}_{1-x}\mathrm{N}$ alloys obtained using Eqs. (1)–(2) and (4). In both figures, we have included the curves (dotted lines) showing dependence of R_c on composition when the Vegard-like rule for C_{ij} (i.e., $b_{ij} = 0$) is assumed. One can see that in $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}$ alloys, R_c changes superlinearly with x for uniform distribution of In atoms, whereas it shows sublinear dependence when In atoms are grouped in clusters or the Vegard-like rule for C_{ij} is taken into account. In the case of $\mathrm{In}_x\mathrm{Al}_{1-x}\mathrm{N}$, R_c shows linear dependence on x in uniform alloys, whereas it changes sublinearly in clustered alloys or when the Vegard-like rule for C_{ij} is assumed. Thus, we find that similarly to composition dependence of ν_c, the In clustering influences significantly the values of R_c in both $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}$ and $\mathrm{In}_x\mathrm{Al}_{1-x}\mathrm{N}$ alloys.

5. Conclusions

In conclusion, we have presented theoretical results showing that Poisson ratio determined for $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}$ and $\mathrm{In}_x\mathrm{Al}_{1-x}\mathrm{N}$ alloys subjected to a uniaxial stress parallel to the c axis of the wurtzite structure shows significant superlinear dependence on composition. The superlinear bowing in Poisson ratio is enlarged by the effect of In clustering. The biaxial relaxation coefficient determined for $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys subjected to a biaxial stress in the plane perpendicular to the c axis of the wurtzite structure changes superlinearly in $In_xGa_{1-x}N$ and linearly in $In_xAl_{1-x}N$. The effect of In clustering results in sublinear dependence of the biaxial relaxation coefficient in both $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys.

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