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Structural and Elastic Properties of Wurtzite Al-Rich $In_xAl_{1-x}N$ Alloys

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We present theoretical study of lattice parameters and elastic constants of wurtzite Al-rich $In_xAl_{1-x}N$ (x = 0.125, 0.1875 and 0.25) alloys using self-consistent *ab initio* calculations with a supercell model. Two different atomic arrangements have been considered for a given x, by either distributing the In atoms as uniformly as possible over the supercell or by clustering the In atoms together in a small part of the supercell. Our calculations reveal that the a and c lattice parameters show almost linear dependence on composition for the alloys with uniform distribution of In atoms, while for the case of alloys with clustered In atoms the c lattice parameter deviates from linearity quite significantly. For the alloys with clustered In atoms, we observe that the values of C_{11}, C_{12}, and C_{44} elastic constants are significantly smaller than the linear interpolated values between the elastic constants of AlN and InN, and the values of C_{33} elastic constant are significantly larger than the corresponding interpolated values. For the alloys with uniform distribution of In atoms, only C_{11} elastic constant deviates significantly from linear dependence on composition.

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1. Introduction

Wurtzite Al-rich $In_xAl_{1-x}N$ alloys are a new and very promising material for application in electronic and optoelectronic devices [1]. In particular, possibility of lattice matching of the $In_xAl_{1-x}N$ alloy with In content $x \approx 0.17$ to GaN allows fabrication of many GaN-based devices, such as distributed Bragg reflectors, intersubband photodetectors and high electron mobility transistors without any mechanical strain in the structure [1]. On the other hand, $In_xAl_{1-x}N$ alloys are interesting also from a basic research point of view, since due to large difference in ionic sizes, one can expect unusual nonlinear dependences of physical properties on In composition [2].

2. Computational method

In this work, we investigate structural and elastic properties of $In_xAl_{1-x}N$ alloys using self-consistent *ab initio* calculations with a supercell model. The indium concentrations, x = 0.125, 0.1875 and 0.25 have been realized by substituting 2, 3, and 4 Al atoms by In in a 32-atom supercell [3]. Two different atomic arrangements have been considered for a given x, by either distributing the In atoms as uniformly as possible over the supercell (uniform alloy) or by clustering the In atoms together in a small part of the supercell (clustered alloy) [3]. Particularly, in an example of a uniform $In_{0.25}Al_{0.75}N$ alloy, In atoms are distributed in such a way that to each N atom belongs one In and three Al neighbors. In the case of a clustered $In_{0.25}Al_{0.75}N$ alloy, every fourth cation hexagonal layer consists of entirely In atoms. Uniform and clustered configurations for $In_xAl_{1-x}N$ alloys with $x = 0.125$ and 0.1875 have been obtained from $In_{0.25}Al_{0.75}N$ alloys by replacing one or two In atoms by Al, respectively. Then, the structures of $In_xAl_{1-x}N$ have been optimized by minimization of the total energy with respect to volume and shape of the supercell. Finally, the supercells have been subjected to test distortions grouped in five sets in order to determine the values of elastic constants for the wurtzite structure [4]. The total energy calculations have been performed using the VASP package which is a plane-wave pseudo-potential implementation of the density-functional theory [5].

TABLE

The values of lattice parameters and elastic constants obtained for $In_xAl_{1-x}N$ alloys with uniformly distributed In atoms and clustered In atoms (in brackets). The results obtained for InN and AlN are also included.

	a [Å]	c [Å]	C_{11} [GPa]	C_{12} [GPa]	C_{13} [GPa]	C_{33} [GPa]	C_{44} [GPa]
$In_{0.125}Al_{0.875}N$	3.1452 (3.1388)	5.0569 (5.0616)	343 (358)	139 (132)	106 (116)	347 (368)	100 (99)
$In_{0.1875}Al_{0.8125}N$	3.1655 (3.1617)	5.0929 (5.1175)	342 (346)	131 (124)	117 (120)	353 (374)	96 (90)
$In_{0.25}Al_{0.75}N$	3.1893 (3.1874)	5.1323 (5.1912)	337 (324)	136 (122)	117 (106)	341 (357)	92 (81)
InN	3.5117	5.6702	229	116	97	239	50
AlN	3.0892	4.9458	397	145	115	371	115

3. Results and discussion

In Table, we show the values of lattice parameters a and c and elastic constants C_{11}, C_{12}, C_{13}, C_{33} and C_{44} obtained for $In_xAl_{1-x}N$ alloys with uniformly distributed In atoms and clustered In atoms (in brackets) in the supercells. One can see that clustering of In atoms modifies both the lattice parameters and the elastic constants of $In_xAl_{1-x}N$ alloys. In order to discuss this effect in more detail, let us focus on the deviations of the lattice parameters (Δa and Δc) and the elastic constants (ΔC_{ij}, $(ij) = (11)$, (12), (13), (33), and (44)) from the linear dependence on alloy composition. Particularly, we define $\Delta a, \Delta c$ and ΔC_{ij} as differences between the values determined from supercell calculations and the values found from the linear interpolation between the results for AlN and InN (also included in Table).

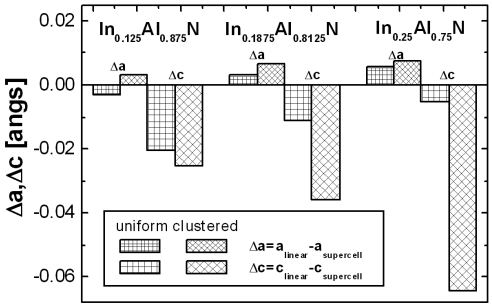

Fig. 1. The values of Δa and Δc for $In_xAl_{1-x}N$ ($x = 0.125$, 0.1875 and 0.25) alloys with both uniformly distributed and clustered In atoms.

In Fig. 1, we show Δa and Δc for $In_xAl_{1-x}N$ alloys with both uniformly distributed and clustered In atoms. One can see that the deviation from linearity for the a lattice parameter is much smaller than for the c lattice parameter. Interestingly, Δc significantly increases with In content for the alloys with clustered In atoms. Figure 2 shows the values of ΔC_{ij} for the considered $In_xAl_{1-x}N$ alloys. We note that (i) ΔC_{11} are significant for the alloys with uniformly distributed and clustered In atoms, (ii) ΔC_{12} and ΔC_{44} are significant for the alloys with clustered In atoms, (iii) ΔC_{33} are also significant but negative for the alloys with clustered In atoms, (iv) ΔC_{13} are relatively small and lie in the computational error range.

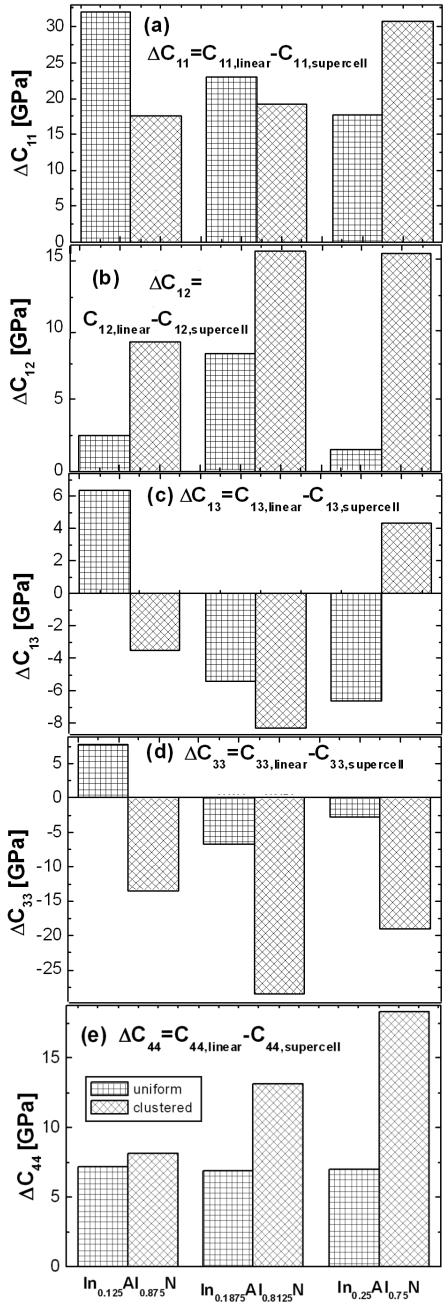

Fig. 2. The values of ΔC_{11} (a), ΔC_{12} (b), ΔC_{13} (c), ΔC_{33} (d), and ΔC_{44} (e) for $In_xAl_{1-x}N$ ($x = 0.125$, 0.1875 and 0.25) alloys with both uniformly distributed and clustered In atoms.

4. Conclusions

Concluding, our calculations reveal that the a and c lattice parameters show almost linear dependence on composition for the alloys with uniform distribution of In atoms, while for the case of alloys with clustered In atoms the c lattice parameter deviates from linearity quite significantly. For the alloys with clustered In atoms, we observe that (i) the values of C_{11}, C_{12}, and C_{44} elastic constants are significantly smaller than the linear interpolated values between the elastic constants of AlN and InN, (ii) the values of C_{33} elastic constant are significantly larger than the corresponding interpolated values. For $In_xAl_{1-x}N$ alloys with uniform distribution of In atoms, only C_{11} elastic constant deviates significantly from linear dependence on composition. Further theoretical studies of the influence of indium segregation on elastic properties of $In_xAl_{1-x}N$ alloys are needed. This refers particularly to the case of the alloys with In content larger than 0.25, which have not been considered

here. Another issue is the usage of the cluster expansion approach with a few different configurations of In atoms in a supercell [6].

Acknowledgments

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