materials design

APPLICATION NOTE

Structure and Elastic Properties of $In_xGa_{1-x}N$

In the design of substrates for the epitaxial growth of $In_xGa_{1-x}N$ alloys it is useful to know the elastic properties of the semiconductor as a function of composition. This application note shows the use of MedeA with VASP 5.2 and the mechanical-thermal (MT) module in computing these properties. Judging by the results for the binaries GaN and InN, the level of accuracy is comparable with that achieved in experiments.

Keywords: Computation, mechanical properties, elastic coefficient, GaN-InN alloys

Experimental Facts

$In_xGa_{1-x}N$ alloys are important optoelectronic materials due to their direct band gap in the blue region of the visible electromagnetic spectrum. The wavelength of emitted light can be tuned by the ratio between Ga and In.

At ambient conditions both GaN and InN crystallize in the hexagonal wurtzite structure as shown in Fig. 1.

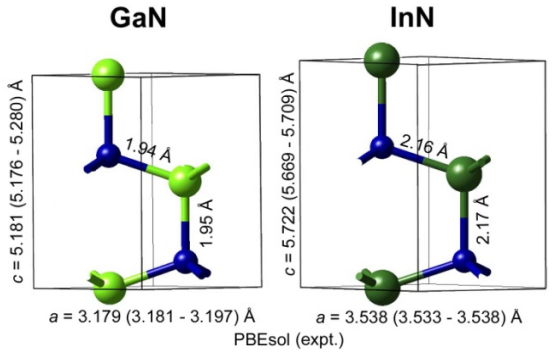

Figure 1. Computed and experimental lattice parameters and bond distances of GaN and InN. The experimental data are taken from the ICSD and Pearson's crystallographic databases.

Computed Results

Using the PBEsol semi-local exchange-correlation potential [1] and the S500 parameter setting in MedeA-VASP, the computed lattice parameters are in remarkable agreement with experiment for both GaN and InN. For GaN the computed value for the lattice parameter *a* is 3.179 Å, which is just slightly below the experimental range of 3.181 – 3.197 Å. The computed lattice parameter *c* of 5.181 Å falls into the experimental range of 5.176 – 5.280 Å. In the case of InN the computed values are also within the experimental range, albeit more on the longer side. It should be noted that this comparison is not completely consistent since the computed values do not contain any temperature effect whereas the experimental data are typically obtained at room temperature.

A model structure and computed lattice parameters of an $In_{0.125}Ga_{0.875}N$ are shown in Fig. 2.

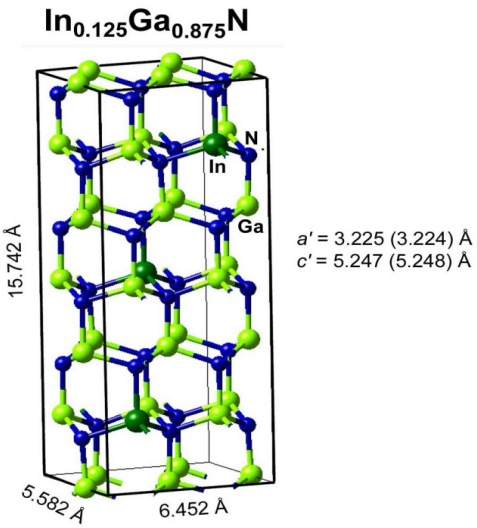

Figure 2. Computed lattice parameters of an In-Ga-N supercell. The values *a'* and *c'* are the lattice parameters backfolded to those of a hexagonal unit cell (values in parenthesis are from Vegard's law).

Table 1. Elastic coefficients and moduli for hexagonal GaN, InN, and $In_{0.125}Ga_{0.875}N$. Experimental values (in parentheses) are from http://www.ioffe.ru/SVA/NSM/Semicond/. The indices *i,j* (1,…,6) denote the sequence *xx,yy,zz,yz,xz,xy*. All values in GPa.

	GaN	**InN**	**$In_{0.125}$ $Ga_{0.875}N$**	
	computed (expt)	computed (expt)	computed	linear interpolation
C_{11}	351 (390±15)	221 (190±7)	316	335
C_{12}	142 (145±20)	120 (104±3)	124	139
C_{13}	106 (106±20)	95 (121±7)	89	105
C_{22}			315	
C_{23}			91	
C_{33}	397 (398±20)	232 (182±6)	349	376
C_{44}	93 (105±10)	47 (10±1)	81	87
C_{55}			81	
C_{66}			95	
Bulk modulus	201 (210±10)	144 (140)	176	194
Young's modulus	271	141	241	255
Shear modulus	106	53	95	99

It is remarkable that the computed lattice parameters are very close to the values obtained from a simple linear interpolation between GaN and InN, *i.e.* by applying Vegard's law.

Of course, this is just one of many possible distributions of In and Ga atoms in a wurtzite lattice. A more detailed modeling of the alloy could be obtained by using a larger supercell and exploring a range of different configurations. In reality, the distribution of the cations in this alloy depends on the conditions in the deposition process and subsequent annealing.

With these caveats in mind, let us investigate the elastic coefficients of these three systems, namely pure GaN, pure InN, and the alloy model.

The computed elastic coefficients and moduli are listed in Table 1. The computed values agree rather well with experimental data, as has also been found for a number of different inorganic crystalline systems (see other Application Notes on elastic coefficients).

Again note that the computed values do not contain effects due to thermal expansion, which are present in the experimental data taken at room temperature. Inclusion of thermal expansion would reduce the computed values.

As expected, GaN is stiffer than InN and the values of the alloy are between those of the binaries. Due to the lower symmetry of the supercell for the alloy there are additional elastic coefficients in the fourth column, which can be backfolded to the hexagonal cell, *e.g.* C_{22} should equal C_{11} and C_{23} should equal C_{13}. Within the numerical uncertainties this is clearly the case.

It is interesting that the computed elastic coefficients and moduli are systematically smaller than values obtained by linear interpolation, as can be seen by comparing the last two columns. This is different from the lattice parameters, where Vegard's law applies well for this class of ternary III-V semiconductors.

Significance

First-principles calculations provide an efficient way to obtain elastic coefficients for semiconductor alloys and other doped systems. Such calculations are probably much faster and more cost effective than experiments.

MedeA modules used for this application

- MedeA framework including crystal structure builders and geometric analysis tools
- JobServer and TaskServers
- InfoMaticA with structural databases (ICSD, Pearson)
- VASP 5.2 and its graphical user interface as integrated in MedeA.
- The MedeA-MT module for the calculation of mechanical and thermal properties

References

1. "Restoring the Density-Gradient Expansion for Exchange in Solids and Surfaces", J. P. Perdew, A. Ruzsinszky, G. I. Csonka, O. A. Vydrov, G. E. Scuseria, L. A. Constantin, X. Zhou, and K. Burke, Phys. Rev. Lett. **100**, 136406 (2008)

For further information please contact

Materials Design, Inc.
T +1 760 495-4924
F +1 760 897-2179
info@materialsdesign.com
www.materialsdesign.com