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The Effects of pressure on wide bandgap GaN semiconductors

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Gallium nitride (GaN) is a group-III nitride semiconductor; which may prove useful in developing optical instruments that operate under high ambient pressures. The purpose of this project is to examine the properties of GaN under varying conditions. The methods used in this experiment consist of modeling free energy as a function of lattice constants; calculating bond lengths, bond strengths, and bulk moduli; and comparing the resultant data with values in published literature. We will also compare these results with experimental data drawn from x-ray diffraction scans. By doing so, we hope to determine whether gallium nitride is suitable for use as a semiconductor at high pressures.

The Effects of Pressure on Wide Bandgap GaN Semiconductors

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ABSTRACT Gallium nitride (GaN) is a group-III semiconductor, which may prove useful in developing optical devices that operate under high pressure or high temperature. The purpose of this project is to examine the properties of GaN at different pressure. The method used in this theoretical study is based on the density-functional theory as implemented in the Vienna ab-initio stimulation package (VASP). Relative phase stability of three experimentally proposed structures; Zinc-blende (zb), wurzite (wz) , and rocksalt (NaCl) are investigated by calculating free energy as a function of the lattice constant. The results obtained in this study can be compared with values in literature, presently available. The curves of pressure versus volume compression are evaluated and compared with experimental data obtained from x-ray diffraction patterns. By doing so, we hope to determine whether gallium nitride is suitable for optical device application at high pressures.

METHODS

The standard density-functional theory [1] is used in carrying out total energy calculations, as implemented in the VASP software. The generalized gradient approximation of Perdew et al. [2] is adopted in the construction of the exchange and correlation interaction.

A total of 8 atoms waere included in rocksalt (NaCl) and zincblende (zb) unit cells. A total of 4 atoms were included in wurtzite (wz) unit cell. Convergence tests with respect to the number of k-points in the Brillouin zone and energy cutoff were performed in this study. For all the calculations presented here, we have used a cutoff energy of 300 eV. The k points are sampled in the Brillouin zone under the Monkhorst-Pack [3] grid of 11x11x11.

A set of equations in thermodynamics was applied to calculate pressure, volume, and enthalpy of NaCl, wz, and zb-GaN strcutures. These are required in order to ultimately calculate a bulk modulus. Data obtained was also compared to articles presently available.

RESULTS AND DISCUSSION

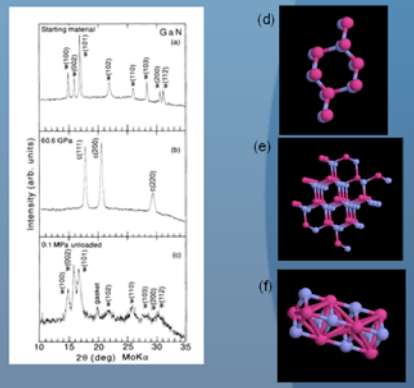

Fig. 1. X-ray-diffraction pattern of GaN (a-c) [4] and crystalline structures of the three polytypes of GaN: (d) *wz*-GaN, (e) *zb*-GaN, and (f) *NaCl*-GaN. The pink and blue spheres represent Ga and N atoms, respectively.

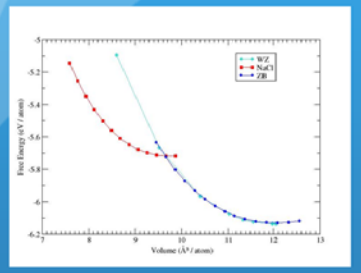

Fig. 2. Energy-volume curves of *wz*-, *zb*-, and *NaCl*-GaN strcutures.

Energetically, the wurtzite structure (WZ) appears to be the most stable structure, as shown in Fig. 2, implying two possible structural changes: (i) a temperature-driven phase transition from WZ to ZB-GaN structure, and (ii) a pressure-driven phase transition from WZ to NaCl-GaN structure.

The calculated volume ccmpression data are in good agreement with experimental data as shown in Fig. 3. In their work. Ueno *et al.* [4] observe that GaN undergoes a monotonous decrease in relative volume with increasing pressure until 52.2 GPa, when the volume of their GaN sample almost immediately falls 17.9%. In comparison, the calculated volume collapse from wz to NaCl strcuture at 52.2 GPa is 20.9% in this work The slight difference may be accounted to the fact that wz begins to transition into the rocksalt phase prior to this point (beginning at ~32 GPa, as shown in Figure 4.

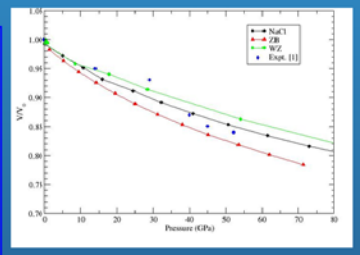

Fig.3 Volume-pressure curves.

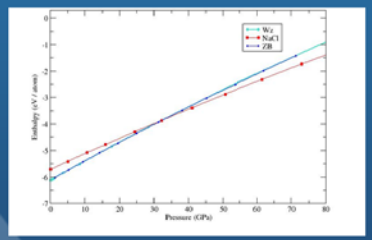

Fig. 4 Enthalpy vs. pressure diagram .

	Lattice constant at equilibrium (angstrom)		Free energy (eV)
	this work	Experiment [5]	
WZ	3.246	3.18	-24.541505
ZB	4.59	4.497	-49.04419
NaCl	4.29	4.225	-45.740401

Table 1 The structural properties of GaN.

According to the enthalpy-pressure diagram, the phase transition occurs from wz-GaN to NaCl-GaN at 32 GPa, as shown in Fig. 4. Based upon our results, then, we expect GaN to exist primarily as wurtzite at ambient pressures, as it is the most stable structure. As pressure approaches the crossover point at ~32 GPa, wurtzite lattices begin to transition into the rocksalt phase; beyond the crossover point, the rocksalt lattice is significantly more stable, dominating the lattice population within the high pressure regime. This corroborates experimental data presented by Ueno *et al.* [4], who demonstrate that (i) this transition occurs regardless of the direction of pressure variation; (ii) the mixture of wz-GaN and NaCl-GaN structures are observed in the x-ray diffraction spectra at 37 GPa; (iii) wz-GaN which has transitioned into the rocksalt phase at high pressures will resume the wurtzite configuration once the pressure has been released, as in Fig. 1 (a-c).

CONCLUSION

- WZ-GaN and ZB-GaN are the most stable polytypes at ambient pressures.
- WZ lattices begin to transition into the NaCl polytype as pressure increases, beginning at ~32 GPa and completing at ~32 GPa
- Theoretical calculations corroborate experimental evidence that sample volume collapses at ~52.2 GPa due to sudden near-complete transition of WZ to NaCl lattices.

FUTURE DIRECTIONS

The next step required is to calculate the bond length, bond strength, and bulk modulus. In addition, further progression would also allow us to calculate the electronic band structures including their energy band gap at several pressure points. which would determine if gallium nitride is a suitable semiconductor under high pressure.

REFERENCES

- Hohenberg and W. Kohn, Phys. Rev. 136, B864, (1964); W.Kohn and L. Sham, Phys. Rev. 140, A1133 (1965).
- J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).
- J. Monkhorst and J. D. Pack, Phys. Rev. B **13**, 5188 (1976).
- Ueno, M., Yoshida, M., and Onodera A., Phys. Rev. B 49, 14 (1994).
- A. Mele *et al*, Internaticnal Journal of Photoenergy, Vol. 3, 111 (2001).
- J. Serrano, A. Rubio, E. Hernandez, A. Munoz, and A. Mujica, Phs. Rev. B **62**, 612 (2000).

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