B3-B1 phase transition in GaAs: A Quantum Monte Carlo Study

C N M Ouma [1, 2], M Z Mapelu [1], G. O. Amolo [1], N W Makau [1], and R Maezono [3],

[1] Computational Material Sciences Group, Chepkoilel University College, Department of Physics , P. O. Box 1125, Eldoret, Kenya

[2] University of Pretoria, Department of Physics

[3] School of Information Science, Japan Advanced Institute of Science and Technology, Asahidai 1-1, Nomi, Ishikawa 923-1292, Japan

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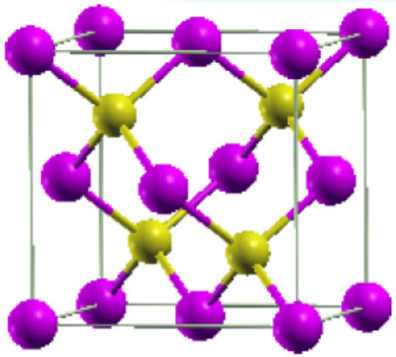
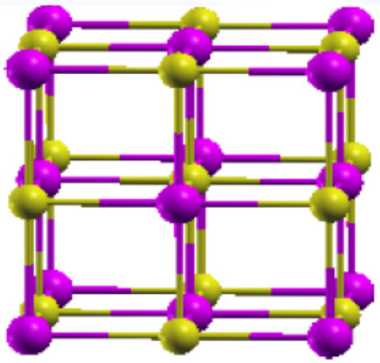
Pressure Induced Phase Transitions

- Diamond Anvil Cell (DAC) technique and the study of high-pressure behavior of many materials.
- Materials exhibit new and interesting phase transitions and novel elastic behavior when under pressure (*Singh and Sadhna 1989*).
- When hydrostatic pressure is increased, a range of behaviors is seen.
- Numerous theoretical and experimental work on high pressure phases
- Rekindling greater interest in this field.

GaAs Pressure Induced Phase Transitions

- Experimental and theoretical investigations have successfully identified high-pressure phases of semiconductors.
- Gallium Arsenide (GaAs) high-pressure phases has been the subject of many speculations (*Durandurdu and Drabold 2002*)
- Experiments and *ab initio* studies reported varying transition pressure values





GaAs Pressure Induced Phase Transitions: Experimental Studies

- Single-crystal X-ray diffraction, X-ray absorption spectroscopy, and elastic neutron scattering to further investigate this structural transformation in GaAs.

- Besson *et al 1991*. B3-B1 occur at 11.5-13.5 Gpa

- Weir *et al* 1989. B3-B1 occur at 17 GPa

GaAs Pressure Induced Phase Transitions: Theoretical Studies

- *Ab initio* DFT Studies using LDA and PBE-GGA pseudopotentials have found different transition points for B3-B1
- Gupta *et al 2008* found B3-B1 occur at about 10.5 Gpa
- Lai-Yu *et. al* 2006 found B3-B1 occur at 16.3 GPa
- Molecular dynamics study by Jose *et al* 2002 found B3-B1 occur at 17GPa

Ab initio Studies

- DFT is an **exact** theory anchoring on the fact that ground state properties can be obtained from *functionals of charge density alone*

- But there is ***no known universally true XC functional***

$$E[n(\mathbf{r})] = T_s[n(\mathbf{r})] + \frac{1}{2}\int\int \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}\,d\mathbf{r}' + E_{XC}n(\mathbf{r}) + \int n(\mathbf{r})\,V_{ext}(\mathbf{r})\,d\mathbf{r}$$

Ab initio Studies: XC Functionals

- Local density approximation (LDA) functionals: based on DMC
- Generalized gradient approximations (GGA) functionals: gradient expansions
- These local and semi-local functionals **have been found to possess significant self-interaction errors**
- Hybrid functionals: **exact exchange**

Quantum Monte Carlo (QMC)

- Continuum Quantum Monte Carlo (QMC) technique (Stochastic)
- QMC ***overcomes some of the failures of DFT***. *Leung(1999),Hood(2003),Healy(2001),Filippi(2002) and Williamson (2002)*
- The two QMC methods; variational Monte Carlo (VMC) and diffusion Monte Carlo (DMC)
- Trial wavefunctions are of central importance in VMC and DMC calculations

Computational Method

- Norm conserving pseudopotentials were used to perform pseudoatomic calculations.
- Quantum Espresso code and CASINO code
- Plane-wave cut-off energy of 60 Ry was chosen and k-point (n=8) meshes were chosen
- All the QMC calculations were performed using 128 atoms.
- Bulk properties : Vinet EOS

Computational Method: QMC

- DFT plane waves are obtained form DFT calculations
- The DFT plane waves are converted in blip waves so as to speed up the calculations
- Optimization of the Jastrow parameter

$$\Psi_{SJ}(\mathbf{R}) = e^{J(\mathbf{R})} det[\Psi_n(\mathbf{r}_i^{\uparrow})] det[\Psi_n(\mathbf{r}_j^{\downarrow})]$$

- VMC calculation

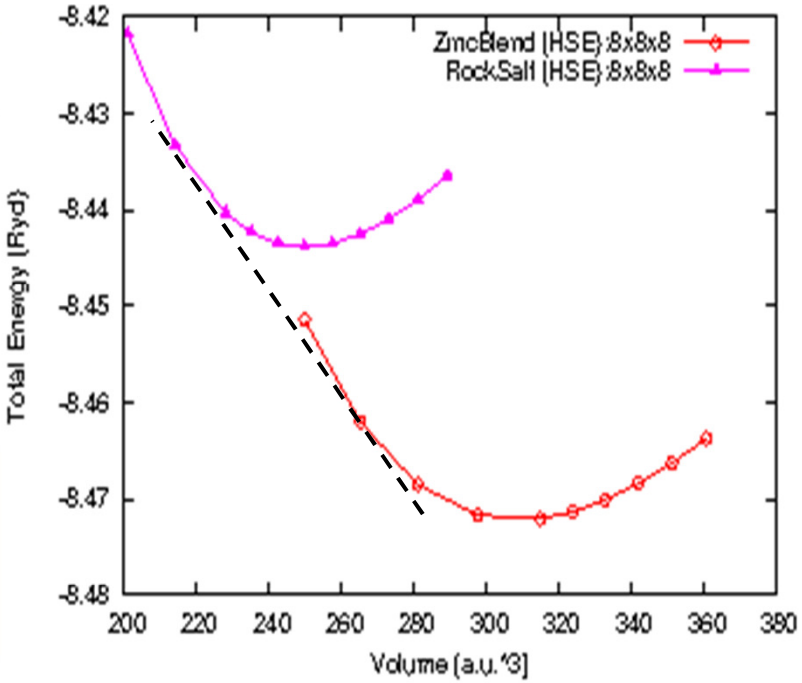
$$E_V = \frac{\int \Psi_T(\mathbf{R}) \hat{H} \Psi_T(\mathbf{R}) d\mathbf{R}}{\int \Psi_T^2(\mathbf{R}) d\mathbf{R}},$$

- DMC Calculation

$$-\frac{\partial}{\partial t}\Phi(\mathbf{R},t) = (\hat{H} - E_T)\Phi(\mathbf{R},t)$$
$$= (-\frac{1}{2}\bigtriangledown_R^2 + V(\mathbf{R}) - E_T)\Phi(\mathbf{R},t),$$

Computational Method

- The transition pressure were obtained via the common tangent method of the carves since



$$P = -\left(\frac{\partial E}{\partial V}\right)$$

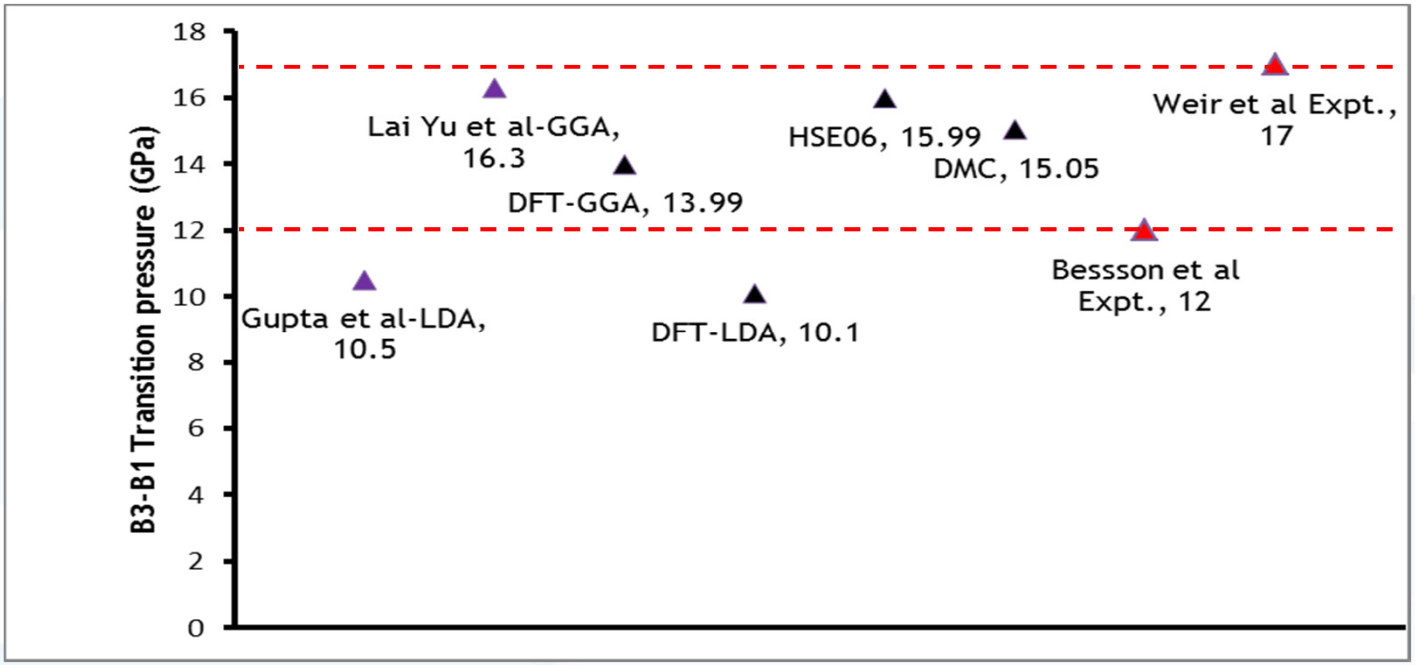
Figure 2. graph showing E-V data obtained by HSE06

Results: Bulk Properties

		a(Å)	B_o(GPa)	B'_o
B3	Present work LDA	5.53	69.16	4.5
	Present work GGA	5.74	66.19	4.7
	Present work HSE06	5.67	73.8	4.3
	Present work DMC	5.65	72.8	4.2
	Other Calculations	5.56a, 5.648b	79.75a, 76.03b	3.5a, 3.9b
	Experiment.	5.653c	75.7c	4c
B1	Present work LDA	5.63	82.95	4.3
	Present work GGA	5.72	78.26	4.3
	Present work HSE06	5.29	90.4	4.2
	Present work DMC	5.27	87.3	4.3
	Other Calculations	5.28a, 5.31b	69.95a, 95.63b	4.87a, 4.05b

a Ref[12],b Ref [11],c Ref [39]

Results: B3-B1 Phase Transition Pressures



	B3 to B1 Phase transition(GPa)			
	GGA	LDA	HSE06	DMC
Present work	13.99	10.1	15.99	15.05±0.15
Other Calculations	16.3	10.5		
Experiment.	17	12±1.5		

Conclusions

- Hybrid functionals and QMC methods present an accurate tool for calculation of phase transition pressures.
- The choice of XC functional is also important in the calculations of transition pressures.
- Further studies however need to be done in controlling the finite-size effects in HSE06 and DMC.

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