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Investigations of Structural Parameters of ZrN

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ABSTRACT The present paper discusses the structural properties of ZrN in B1, B2 and B3 phase by using the hybrid scheme B3LYP as in inbuilt crystal code. The code is based on well-known theory of the density functional theory. The lattice constant and the bulk modulus are calculated and compared with the previous investigation

KEYWORDS DFT, Crystal06, ZrN, B3LYP

INTRODUCTION

High Refractory metal nitrides have diverse application likewise in magnetic application, tools used for cutting, optical cutting, fuel cells, working at lower temperature. Several studies, using different types of techniques and methods have been reported so far in various metals nitrides such as TiN, ZrN, HfN. The review of literature confirms that, very few studies have been reported on B3 phase and to the best of knowledge, no one has used LCAO method.

Hence, in the present paper an attempt has been made to carry out structural investigations of ZrN in B1, B2, and B3 Phase

METHODOLOGY

The density functional theory (DFT) has been used to investigate the properties of ZrN using the hybrid scheme B3LYP as inbuilt in crystal code. For making the program, the basis Gaussian basis set of Zr and N have been used, The lattice constant and bulk modulus are computed for the ZrN in three phases, B1, B2 and B3.

RESULTS AND DISCUSSION

The properties in B1, B2, B3 phase have been calculated by the finding the total energy with respect to the variation of the volume of the primitive cell of the crystal. In order to find the lattice constant, the minimum energy is observed and the corresponding to this energy represents the minimum volume which further highlights the lattice constant. For ,finding the bulk modulus, and the pressure derivative of bulk modulus the calculated energies are fitted to BrichMrughman equation of state. Figure 1-3 represents the curve of ZrN in B1, B2 and B3 phase respectively. The calculated values are compared with other values in the Table 1

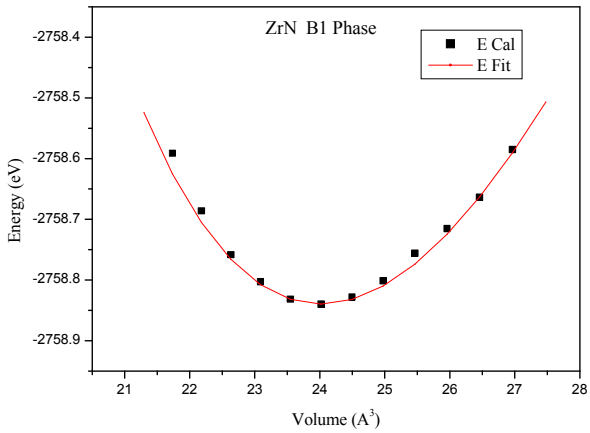

Figure 1: E vs V ZrN B1 Phase

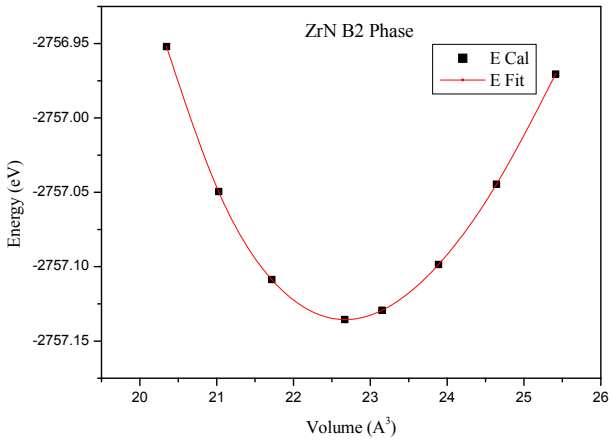

Figure 2: E vs V ZrN B2 Phase

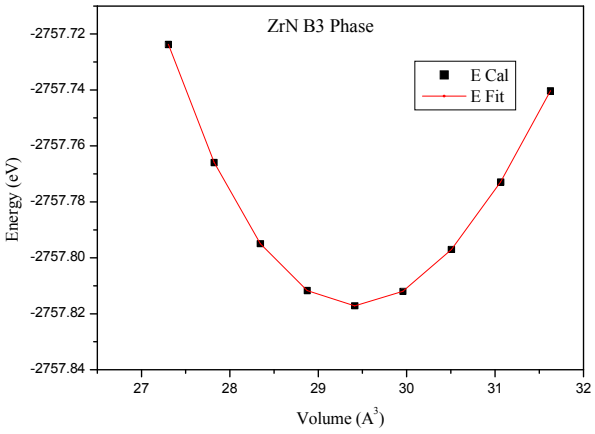

Figure 3: E vs V ZrN B3 Phase

Table 1 Structural Parameters of ZrN in B1, B2, B3 Phase

	A			B			B′		
	B1	**B2**	**B3**	**B1**	**B2**	**B3**	**B1**	**B2**	**B3**
Present	4.58	2.82	4.9	268	199.5	170.5	3.56	2.93	3.23
Experimental (R.W.G. Wyckoff.)	4.61								
(A.N. Christensen,)				215					
Z. Wu et al.	4.52			285					
W. Chen and J.Z. Jiang	4.57		4.95	248					
A. Srivastava and B. D. Diwan	4.561	2.88	4.93	231.74	193.54	158.60	3.23	2.79	3.19

CONCLUSION

In summary, the LCAO, method has been used to investigate the structural parameters of ZrN using density functional theory, it was observed that as the phase changes from B1 to B3 the lattice constant values are 4.58, 2.82 and 4.9 respectively. In context to bulk modulus, the variation is from 268 to 170.5 as the phase changes from B1 to B3. The calculated values are in close proximity with the previous agreement.

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