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First Principle Study of Pressure Induced Phase Transition in Arsenic

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Abstract*: In the present work, we report investigation of the crystal structure of arsenic under compression, focusing mainly on the pressure-induced A7 → simple cubic (sc) phase transition. The two-atom rhombohedra unit cell is subjected to pressures ranging from 0 GPa to 50 GPa; for each given pressure, the cell lengths , angles and the atomic positions are allowed to vary until the relaxed structure is obtained. The nearest and next-nearest neighbor distances give indication of the structural phase transition. Calculations are performed using the local density approximation (LDA) and the PBE and PW91 generalized gradient approximations for the exchange-correlation functional using Quantum Espresso. The A7 → sc transition is found to occur at 30GPa-40GPa, no volume discontinuity is observed across the transition in any of the three cases. k-point grids as dense as 8×8×8 enable us to present reliably converged results for the A7 → sc transition of arsenic.

Keywords:* Phase Transitions, Density Functional Theory, Quantum espresso

I. INTRODUCTION

The computational study of high-pressure behaviour of materials provides the ability to properly examine the phase transitions from one structure to another of the material.

The paper is organized as follows. Section II contains the background material that pertains to our study, description of the *A*7 phase, a quick review of the structural transformation that yields the sc phase when a sufficiently high external pressure is applied, In Section III, we mention about the methods that we have followed, In Section IV, we present and discuss our results, and also comparing them with the literature.

At ambient pressures, arsenic is a covalently bonded compound existing in the rhombohedral (A7) phase.

The rhombohedral primitive cell of arsenic contains two atoms and is described by the length of primitive lattice vectors, a, and the angle, α, between each set of primitive lattice vectors, and by the atomic positional parameter, x , which determines the positions of the two atoms along the cell's body diagonal. The sc lattice can be viewed as composed of two face centered cubic (fcc) lattices.. Under high pressures, arsenic undergoes a transition from half metallic A7 to metallic sc.. The pressure induced A7 to simple cubic (SC) transformation in As has been proved DFT. The A7 structure is among several structures favored by the group-V elements, which are variations of the SC structure.

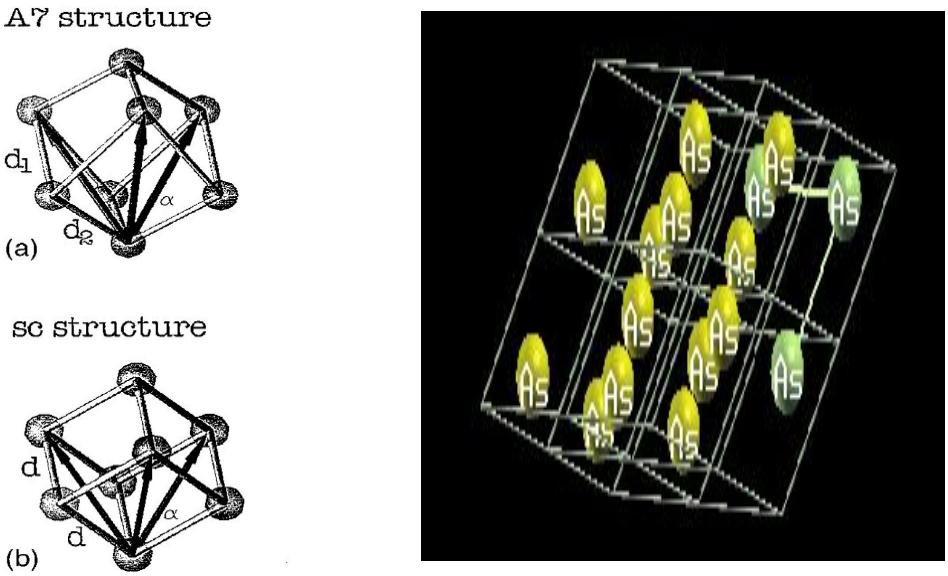

Fig. 1 Arsenic in A7 structure (XcrysDen)

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II. METHODS

We use the QUANTUM ESPRESSO [1] which is a computer package to study the electronic structure and optimization using the molecular dynamics simulation. The Quantum ESPRESSO distribution contains the core packages PW scf (Plane-Wave Self-Consistent Field) and CP (Car-Parrinello) for the calculation of electronic-structure properties within Density-Functional Theory (DFT), using a Plane-Wave (PW) basis set and pseudo potentials. It also includes other packages for more specialized calculations.

We have also used XCrySDen [5] which is a crystalline- and molecular-structure visualisation program. The name of the program stands for Crystalline Structures and Densities and X because it runs under the X-Window environment. It facilitates a display of iso-surfaces and contours, which can be superimposed on crystalline structures and interactively rotated and manipulated. The Structure of As can be seen in Fig(1).

III. RESULTS AND DISCUSSION

We first take an overview of the behavior of the nearest and next-nearest neighbor distances as the pressure is increased from 0 GPa to 50 GPa. It has already been stated that for the A7 → sc phase transition in particular, the behavior of these two quantities gives the clearest indication of when a structural phase transition has occurred. Using QUANTUM ESPRESSO we calculated the lattice parameter, internal coordinate, angle, volume at variable pressures (0-50 GPa), by using the calculated values we plotted the graphs.
Figure 2 reveals that around 30-40 GPa there is a, change in the internal coordinate.
Figure 3 shows that around 30-40 GPa there is a variation in lattice parameter.

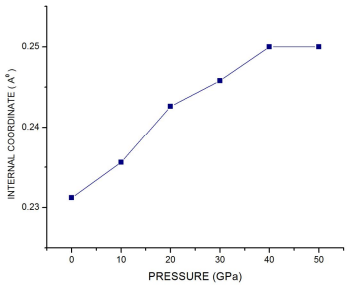

Fig. 2

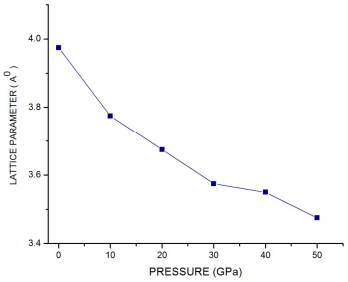

Fig. 3

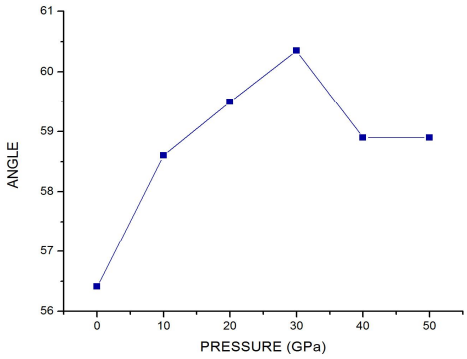

Fig 4

Figure 4 reveals that around 30-40 GPa angle is changing its direction which clearly indicates about the structure transition in Arsenic.
These findings are the indications of A7-SC phase transition occurrence in arsenic between 30-40 GPa. Our results match with the experimental results [2] as provided in the literature as given in Table -1.

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TABLE -1

Calculation (A7)	Angle(α)	Internal Coordinate(A^0)
This Work	56.4	0.231
LAPW [3]	55.9	0.229
PP [3]	56.28	0.23
PP [4]	56.24	0.23

IV. CONCLUSIONS

Thus we have performed first principle studies of the two-atom unit cell of arsenic under compression to investigate its high pressure behavior and compare with experiment. In the context of the A7 → sc transition, our results strongly support the experimental findings [2].

The conclusions being A7 to simple cubic transition of arsenic takes place around the pressure 30-40Gpa. From the graphs which we have plotted we can say that there is no volume discontinuity, so this is a second order transition.

V. ACKNOWLEDGMENT

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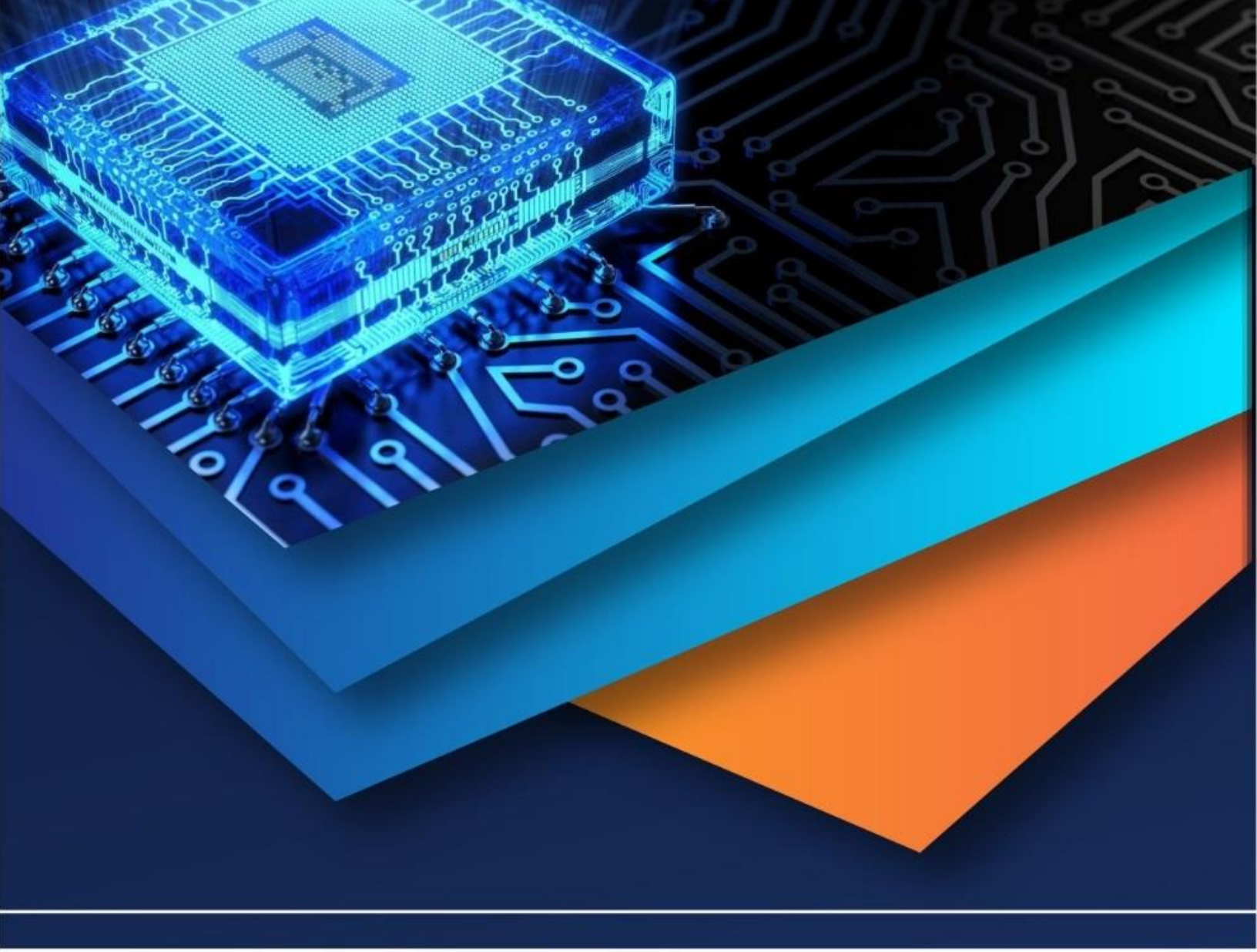

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