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Pressure Dependent Elastic And Mechanical Properties Of Hexagonal Structured Pdh_2

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ABSTRACT

The elastic and mechanical properties of Laves phase PdH_2 compound have been investigated in the pressure range 0-150 GPa. The Lennard- Jones potential model has been applied to compute the second order elastic constants of PdH_2. These elastic constants are found to increase monotonically in the given pressure range .The second order elastic constants are utilized to compute the pressure dependent mechanical constants such as Voigt- Reuss constants (M, C^2), Young's modulus (Y), bulk modulus (B), shear modulus(G)& Possion's ratio (σ). All computed parameters increase symmetrically with the increasing pressure. The results reached at, from the present investigation, have been deliberated upon, and compared with the available data from previous work.

Keywords: elastic properties, mechanical properties, palladium dihydrides.

1. Introduction

Much attention has been focussed on Metal-Hydrides on account of certain fascinating properties, such as high hydrogen-storage capacity, fast hydrogen absorption/desorption, long-term life-cycle and low toxicity [1]. To decipher the bonding mechanism of H atoms with the metal lattice, in general, a special case wherein M=Pd serves the purpose. A study of electronic properties of PdH helps understand other M-H systems [2]. Palladium metal is known to absorb hydrogen at ambient conditions and the dissociative adsorption of H_2 molecules occurs with little or no activation energy barrier on the palladium surface. The reversible hydrogen absorption property can be used for hydrogen storage [3]. Increasing the hydrogen concentration will cause volume expansion of PdHx. Based on this mechanism, a Pd based H_2 sensor was used to measure the hydrogen concentration [4]. Due to the dissociative properties of H, Pd-H can be used for hydrogen-related catalytic reactions [5].The hydrogen storage capability and some other properties , like mechanical and superconducting,

are affected by concentration of absorbed H atoms. [6].It was found that the hydrogen reduces the compression resistance in Pd-H, in which bulk modulus decreases from 195 GPa to 183 GPa with the increase of H concentration from 0 to 0.76 . It has been reported by Greenwood and Earn S haw that the metallic conductivity reduces as hydrogen is absorbed over PdHx, and reduces with the increase of x, until at around $PdH_{0.5}$,the solid becomes a semiconductor [7].Experiments show that PdH_x can be formed on the top of multi-wall carbon nanotubes. For $0 < x < 1$, it is stable in face-centered cubic (fcc) structure. While, for $x = 2$ it has a hexagonal close-packed (hcp) structure. Palladium was studied in a high pressure hydrogen atmosphere up to 20 GPa. However, the PdH_2 was not observed by X-ray diffraction until the pressure up to 20 GPa .

As per author's knowledge, no study has been done on elastic& mechanical properties of PdH_2, which motivates to study these properties of PdH_2 in the pressure, range 0-150 GPa. This study uses Lennard-Jones potential techniques to investigate the elastic& mechanical characteristics. This is used to explain the characteristics of the PdH_2 compound.

2. Theory

The interaction potential model technique is one of the most well-established theories for calculating out the higher order elastic coefficients of hexagonal wurtzite and hcp shaped compounds [9]. By applying the second-order of elastic energy density, the formulations of higher-order elastic constants were determined.

$$C_{ijklmn\ldots} = \frac{\partial^n F}{\partial \eta_{ij}\, \partial \eta_{kl}\, \partial \eta_{mn} \ldots} \quad (1)$$

The second-order (C_{IJ}) elastic coefficients of the hcp material can be written as follows [10]:

$$\left.\begin{array}{ll} C_{11} = 24.1\ p^4 C' & C_{12} = 5.918\ p^4 C' \\ C_{13} = 1.925\ p^6 C' & C_{33} = 3.464\ p^8 C' \\ C_{44} = 2.309 p^4 C' & C_{66} = 9.851\ p^4 C' \end{array}\right\} \quad (2)$$

The Born elastic stability conditions for a single compound of the hcp PdH_2 composite [11] is expressed through:

$$\left\{\begin{array}{c} C_{44} > 0 \\ C_{11} - |C_{12}| > 0 \\ (C_{11} + C_{12})C_{33} - 2C_{13} > 0 \end{array}\right\} \quad (3)$$

The physical properties of compound can be predicted by the B (bulk modulus), G (shear modulus), and Y (Young's modulus) [12, 13]. It is achievable to use bulk modulus to clarify the average atomic bond strength since it is clearly associated to cohesive energy or bond formation energy of atoms in compound. The G is a important factor in determining a compound's hardness. Y is calculated to reveal stiffness of a solid that depends on the strength of its atomic bonds. The B and the G for the hexagonally structured PdH_2 compound can be determined from literature,

$$M = C_{11} + C_{12} + 2C_{33} - 4C_{13}, C^2 = (C_{11} + C_{12})C_{33} - 4C_{13} + C^2{}_{13};$$
$$Y = \frac{9GB}{G + 3B}; \quad B = \frac{B_V + B_R}{2}; \quad G = \frac{G_V + G_R}{2}; \sigma = \frac{3B\text{-}2G}{2(3B + G)} \qquad (4)$$

. Results and discussion

3.1. Elastic and mechanical properties

In this investigation, the elastic constants (six SOECs) have been obtained. The basal plane distance 'a', and axial distance (c/a= p) are given in Fig. 1 [14]. The lennard jones constants (b_0) are 1.63×10^{-62}.

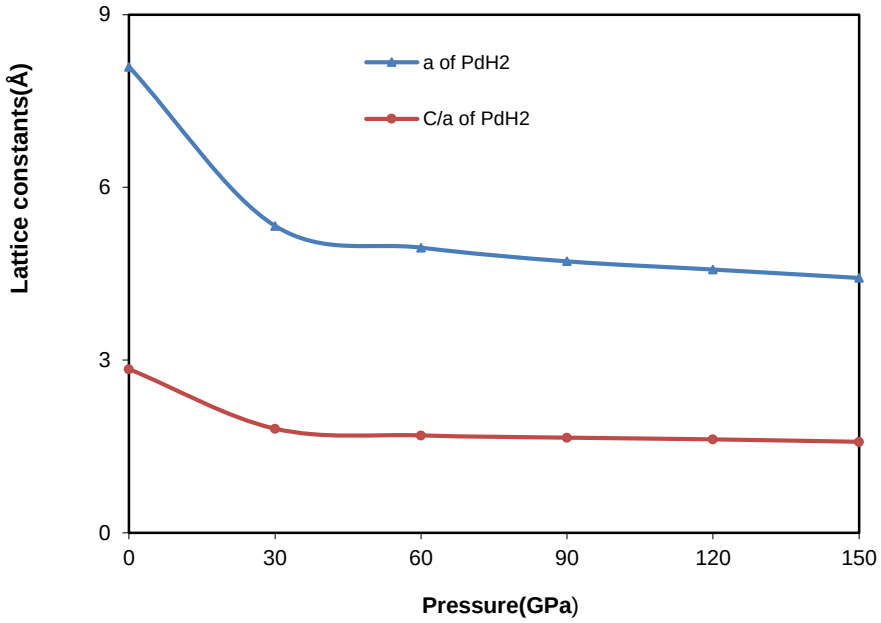

Fig.1. Lattice constants of PdH_2

The computed values of pressure dependent SOECs are displayed in Fig.2. There are six SOEC's. It is observed form Fig.2 that PdH_2 compound's elastic constants increase monotonically as pressure increases. As pressure increases, C_{11} and C_{33} change rapidly, although C_{13}, C_{12}, and C_{44} exhibit a not too rapid variation.

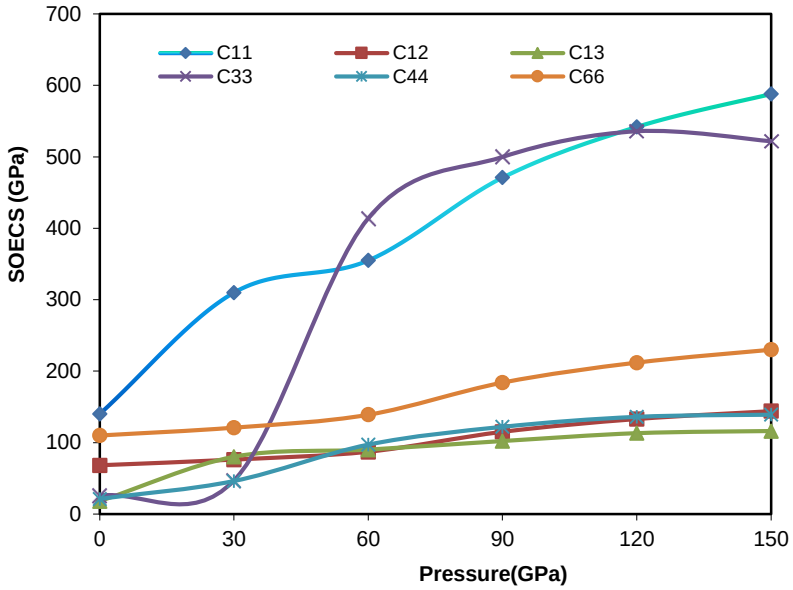

Fig.2.Second order elastic constants of PdH_2

It is possible that PdH_2 compound is mechanically stable as per Born stability criteria using Eq.(3) in the pressure range 0-150GPa. The computed value of pressure dependent Voigt-Reuss constant (M, C^2), bulk modulus (B), shear modulus (G), Pugh's ratio (G/B), and Poisson's ratio (σ) have been computed using Eqs. (4), and, are given in Fig. 3.

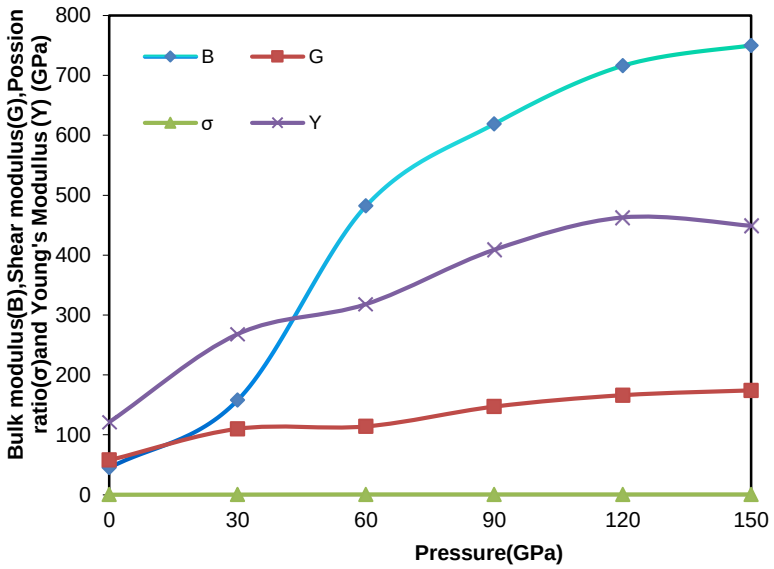

Fig.3. B,G,Y,σ of PdH_2

According to Fig. 3, the bulk modulus B is significantly larger than the shear modulus, G, in the pressure range of 0-150 GPa. The bulk modulus is found to be 45 at 0 GPa, which is comparable with literature [14]. It can be shown form Fig. 3 that B increases with increase in pressure. This shows that material has good hardness.

Table.1. Pressure-dependent M, C^2, B, G, B/G, and σ for PdH_2.

Pressure (GPa)	M	C^2	B	G	B/G
0	172	5660	45	58	0.78
30	412	72858	158	110	1.43
60	397	275646	482	115	4.19
90	493	440496	619	148	4.182
120	524	546653	717	166	4.31
150	528	576984	750	174	4.31

If Pugh's ratio (B/G) is greater than 1.75 then the compound is brittle otherwise, it is ductile [15]. In the present analysis $PdH_2$is found to have the value of B/G greater than 1.75 at 60GPa, hence PdH_2 is ductile in nature, below 60 GPa, as given in Table 1. The value of B/G increases from 0.78 to 4.31 in the pressure range 0 to 150 GPa as per Table 1. The Young's moduli (Y), have been calculated using Eq's (4). The pressure dependent Y is shown in Fig. 3. The Young's modulus measures the stiffness of compound, and the larger its value, the stiffer the compound. The Young's modulus (Y) of PdH_2 increases with increasing of pressure as shown in Fig. 3.

4. Conclusion

The elastic, mechanical and thermo-physical properties of PdH_2 compound were investigated using Lennard-Jones potential technique in the pressure range (0 to 150 GPa) in the present study. The investigation leads to the following conclusion:

- The theory for evaluation of higher-order elastic constants is also suitable for PdH_2 in the pressure region 0-150GPa.
- The stability criteria have been followed by PdH_2, which confirms the stability of the material
- PdH_2 has been found to be ductile in nature on the basis of its Pugh's ratio and Poisson's ratio in the given pressure range.

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Conflict of interest

The authors declare that they have no any known competing of interests in this paper.

References

1. Sakintuna, B., Lamari-Darkrim, F. & Hirscher, M. Metal hydride materials for solid hydrogen storage: a review. Int. J. Hydrog. Energy 32, 1121–1140 (2007).
2. Manchester, F., San-Martin, A. & Pitre, J. Te H–Pd (hydrogen-palladium) system. J. Phase Equilibria 15, 62–83 (1994).
3. Adams, B. D. & Chen, A. Te role of palladium in a hydrogen economy. Mater. Today 14, 282–289 (2011).
4. Fisser, M., Badcock, R. A., Teal, P. D. & Hunze, A. Optimizing the sensitivity of palladium based hydrogen sensors. Sensors Actuators B: Chem. 259, 10–19 (2018).
5. Li, Y. et al. Near-surface dilution of trace Pd atoms to facilitate Pd-H bond cleavage for giant enhancement of electrocatalytic hydrogen evolution. Nano Energy 34, 306–312 (2017).
6. Greenwood, N. N. & Earnshaw, A. Chemistry of the Elements (2nd ed.) (Butterworth-Heinemann, 1997).
7. Ponyatovskiĭ, E., Antonov, V. E. & Belash, I. Properties of high pressure phases in metal-hydrogen systems. Physics-Uspekhi 25, 596–619 (1982).
8. Switendick, A. C. Electronic structure and stability of palladiumhydrogen (deuterium) systems, PdH(D)n, $1 \leq n \leq 3$. J. Less Common Met. 172, 1363–1370 (1991).
9. D. J. Quesnel, D. S. Rimai, and L. P. DeMejo "Elastic compliances and stiffnesses of the fcc Lennard-Jones solid" Phys. Rev. B 48, 6795 ,1993.
10. H. B. Huntington, The Elastic Constants of Crystals (Academic, New York, 1958)
11. Sin'Ko, G. & Smirnov, N. Ab initio calculations of elastic constants and thermodynamic properties of bcc, fcc, and hcp Al crystals under pressure. J. Physics: Condens. Matter 14, 6989 (2002).
12. W. Voight, Lehrbuch der Krystallphysik (Teubner, Leipzig, 1928), p. 962.
13. R. Hill, Proc. Phys. Soc. London Sect. A 65, 349 (1952)
14. Zeliang Liu, Rajeev Ahuja, Huijian Li & Wei Luo "Mechanical and electronic properties of vander Waals layered hcp PdH2" Scientific Reports | (2020) 10:8037.
15. Pugh, S. XCII. relations between the elastic moduli and the plastic properties of polycrystalline pure metals. Te London, Edinburgh, Dublin Philos. Mag. J. Sci. 45, 823–843 (1954).