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Elastic, mechanical, thermo-physical, and ultrasonic investigation in platinum carbide

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ABSTRACT

A comprehensive study of elastic, mechanical, thermophysical and ultrasonic properties of novel platinum carbide (PtC) have been reported. The elastic constants, mechanical properties e.g. bulk modulus, shear modulus, Young's modulus etc., direction dependent thermal and ultrasonic properties of PtC in rock-salt (RS-type) and wurtzite (WZ-type) structures are determined. Thermal properties e.g. thermal relaxation time, lattice thermal conductivity, specific heat per unit volume, crystal energy density, acoustic coupling constants, and ultrasonic attenuation were determined along different directions. In order to access the microstructural information and nature of material the direction dependent ultrasonic properties of PtC were correlated with other thermo-physical properties. The elastic, mechanical, thermophysical and ultrasonic properties of wurtzite crystal structure have been reported for first time. All results reveal that PtC would favour wurtzite crystal phase. The compound is stiffer in wurtzite phase. The obtained results may be further explored for research and industrial applications.

1. Introduction

In last three decades, intensive experimental and theoretical researches have been done on group IV and V transition metal carbides (TMCs) [1–3]. TMCs are the potential candidate for research due to their widespread technological applications in cutting tool and hard coating due to their durability, hardness and great strength [4]. TMCs have also shown interesting superconducting, optoelectronic, semiconducting, and thermal properties [4,5]. Platinum carbide is one of the noble metal carbide belongs to refractory compound very popular among researchers in the last decade [6,7]. Dahliah *et al.* [7] have investigated the structural stabilities of PtC compound in seven different crystallographic phases using full-potential linearized augmented plane wave method based on density function theory. They have reported temperature and pressure dependent variation of thermodynamic properties of PtC and observed that PtC shows metallic behaviour in all phases under study. The enormous mechanical, thermal properties, high thermal conductivity, superior mechanical properties and great hardness are the basic reasons for growing interest in PtCs [8–10]. Recently the structural and mechanical properties of noble metal carbides in different phases have been reported using generalised gradient approximation scheme (GGA) in literature [11]. The rock-salt (RS) structure synthesis reported using X-ray diffraction (XRD) pattern under high temperature and high pressure with large value of bulk modulus [12]. However, it has been reported in literature that the stable structure of PtC is obtained in zinc blende (ZB) structure within low temperature regime [13]. Ab intio study [14] reveals the investigation of electronic and structural properties of low index surfaces i.e. <100>, <110> and <111> surfaces of ZB PtC. Rabah et al. [15] reported the ground state properties of PtC in the, rock-salt (RS), zinc-blende (B3), wurtzite (WZ), nickel-arsenide (B8) and lead (II) oxide (B10) structures using the full-potential linearized muffin-tin orbital method (FP-LMTO) within the local density approximation (LDA) to density-functional theory (DFT) and compared with available experimental and theoretical data. They have also reported that possibility of phase transition from RS-structure to ZB-structure is possible once the pressure reduces to ambient condition. They have predicted that RS-structure is unstable at zero pressure while ZB-structure is stable at ground state. The studies on the ground states,

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