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STUDY OF TUNGSTEN DISULFIDE (WS2) NANOMATERIALS UNDER HIGH PRESSURE

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Abstract:

The present article demonstrates the study of properties as well as applications of tungsten sulfide (WS_2) nanoparticles under high pressure. Here, the detail studies regarding the compression nature of WS_2nanotubes (NT-WS_2). In addition to this, the study of fullerene-like nanoparticles (IF-WS_2) is done with the help of in situ high-pressure X-ray diffraction (XRD) and Raman spectroscopy. After extensive study, outcomes demonstrate that the impacts of size and morphology play important roles in examining the high-pressure behaviour of WS_2 nanoparticles, and consequently, a considerable insight into the relationship between structure and properties was observed.

Key Words: Tungsten Sulfide (WS_2), Nanomaterials, XRD, WS_2 Nanotubes (NT-WS_2), Fullerene-Like Nanoparticles (IF-WS_2).

1. Introduction:

Tungsten disulfide (WS_2) belongs to the class of transition metal dichalcogenides (TMDs) which are two dimentional semiconductor nanomaterials. Previously, several studies regarding high-pressure nano materials have been done and therefore, remarkable interest towards the evaluation of the intriguing properties of these materials under extreme conditionsis emerged [1-3]. As compare to conventional bulk materials, it is observed that the size and shape shows significant impacts in determination of the high-pressure behavior of nanoscale materials [4]. As per reported researches, several of interesting phenomena are observed. In this context, reduction in particle size of CeSe nanoparticles result in increased the phase transition pressure [5], and shape-tuned, high-pressure phase transition sequences for TiO_2nanowires [6] and ZnS nanorods [7] are also observed. However, the impacts of size and morphology on the high-pressure behavior of nanomaterials differ from one system to another. Therefore, more extensive studies are required for establishing the impact of high pressure on different nanomaterials as a function of size and shape, which may be very helpful towards the understanding of the physical and chemical characteristics of nanomaterials.

Basically, transition-metal dichalcogenides (TMDs) are considered as layered materials having chemical formula MX_2, where M stands for transition metal element and X for chalcogen element like sulfur, selenium, tellurium [8-10]. In most of the cases, each layer of layered TMDs exhibits a common X-M-X sandwich structure and chalcogen atoms arranged in hexagonal manner in two planes separated by a sheet of metal atoms. The weakvan der Waals forces are observed in two adjacent layers and hence the crystals are formed in different polymorphs. These crystals show variations in stacking mode and metal-atom coordination [11-12]. Tungsten disulfide (WS_2) belongs to the TMDs family and recently extensive attention towards its structural [13], thermal [14], and optoelectronic [15] properties has been attracted. Therefore, remarkable progress has been observed in precisely monitoring the size and shape of synthesized WS_2nanocrystals via numerous methods, like hydrothermal methods [16], liquid-phase exfoliation [17], pulsed lasers [18], and mechanical activation [19].

Particularly, a successful synthesis ofWS_2nanotubes (NT-WS_2) and fullerene-like nanoparticles (IF-WS_2) have been reported. Due to the specific nested structure and tiny size, NT-WS_2possessedfascinating photovoltaic and other optical properties [20]. IF-WS_2nanoparticles demonstrated solid-state lubrication properties and superior mechanical stability [21]. The aforementioned structure-driven characteristics have attracted considerable interest in high-pressure investigations of these nanoparticles. IF-WS_2possesses great compliance and shock-absorbing property, and has potential to withstand shock pressure of up to 25.0 GPa with mild nano structural degradation [22]. WS_2nanotubes demonstrate structural breakdown perpendicular to the tube direction under high pressure, as well as macroscopic conductivity above the percolation threshold of 9.0 GPa [23]. However, monitoring the high-temperature syntheses of nanomaterials cannot be done easily and, therefore; structural as well as chemical defects are abundant. Hence, information regarding crystal structure is important to investigate intensive understanding of the pressure-property relationship. To achieve above goal, the structure and related mechanical properties of nanomaterial systems under pressure can be examined by high-pressure XRD with the help of diamond anvil cell (DAC). Therefore, important structure-property relationships can be demonstrated via in situ structure and property characterization of nanomaterials.

Herein, a detail study of WS_2nanoparticles having two contrasting particle shapes is reported with the help of in situ high-pressure XRD and Raman spectroscopy. A significant variation in compressibility of IF-$WS_2$and NT-$WS_2$was observed. The different high-pressure property of the IF-$WS_2$and NT-$WS_2$is studied with respect to the effects of shape and size.

In present article, the possible reasons for the difference in compressibility between the NT-$WS_2$and the IF-WS_2 are extensively studied. The aforementioned study shows that the order of their compressibility was found to be as follows NT-WS_2<Bulk WS_2< IF-WS_2. Several literature reports revealed that, at higher pressures, nanomaterials undergo phase transitions as the average particle size decreases and possess greater bulk moduli than those of their corresponding bulk materials. The above observation can be justified as the surface-to-volume ratio of nanoparticles increases; the increase in surface energy is also observed [24-25]. Due to the slender shape of the NT-WS_2, a higher surface-to-volume ratio was observed as compare to bulk materials, which results in better hardness. However, the bulk modulus of the IF-WS_2 demonstrated the contrast result, i.e., its modulus was smaller than that of the bulk 2H-WS_2flakes. It was suggested that the anomaly may have resulted from the particle morphology and the relatively large defect density in the IF-WS_2. In other words, IF-$WS_2$are quasi-nanosphere nanoparticles made up of multiple closed WS_2layers in an onion-like nested arrangement. The weak van der Waals force between the adjacent layers is responsible for more compressibility ofWS_2along the c-axis than along the a-axis. Hence, IF-WS_2 possesses greater compressibility along c-axis. Furthermore, complete seaming of the folded layers along two directions (a- and b-axes) is not possible, leaving many defects in the IF's structure. Factually, the nanotubes are folded along one axis only implies that they can more easily fold and seam and, hence, that their defect density is considerably smaller than that of IF nanoparticles. Due to the high defect density, IF nanoparticles become more prone towards structural distortion under pressure. The uniaxial compression of individual WS_2nanotubes, which also possesses interlayer shearing, was also investigated previously [26]. In case of the IF-WS_2, the interlocking between layers are observed and their potential to shear with respect to each other is more limited; therefore, the potential towards strain absorbance is lower compared to the NT-WS_2. On the basis of above discussion, it is clear that the present study provides a reference to better understand the effects of size and morphology on the high-pressure behavior of WS_2nanoparticles.

4. Conclusion:

In conclusion, the role of in situ high-pressure XRD and Raman spectroscopy was studied for the investigation the high-pressure behavior of WS_2nanotubes (NT-WS_2) and fullerene-like nanoparticles (IF-WS_2). The outcomes demonstrate that the structures of NT-WS_2 and IF-WS_2 remain stable up to 24.0 GPa, showing excellent compression-resisting nature. Hence, NT-$WS_2$and IF-WS_2 can be used as lubricants. The bulk moduli of the IF-$WS_2$and NT-WS_2were found to be 46.3 GPa and 81.7 GPa, respectively, as compare to ≈60 GPa for the bulk material, suggesting a significant difference in the compressibility of the samples. It is also suggested that the surface energy, crystal growth orientation, defect density, interlayer shearing, and nanosize effects play an important role in the high-pressure behaviors of these nanoparticles. The present comprehensive study will be very useful in the design and development of novel functional nanomaterials.

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