Computational Materials Science 151 (2018) 196–203

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Effect of sample size, temperature and strain velocity on mechanical properties of plumbene by tensile loading along longitudinal direction: A molecular dynamics study

Dhiman Kumar Das[a,*], Jit Sarkar[b], S.K. Singh[a]

[a] Department of Mechanical Engineering, Indian Institute of Technology (Indian School of Mines), Dhanbad 826004, Jharkhand, India
[b] Department of Metallurgical and Materials Engineering, Indian Institute of Technology, Kharagpur 721302, West Bengal, India

ARTICLE INFO

Keywords:
Plumbene
Two-dimensional nanomaterials
Molecular dynamics
Mechanical properties

ABSTRACT

In recent years, two-dimensional (2D) nanomaterials have received tremendous attention due to their unique structure and extraordinary properties. Graphene, silicene, germanene and stanene- the 2D allotropes of carbon, silicon, germanium and tin have been reported in last few years and their properties have been studied elaborately. Plumbene, the 2D allotrope of lead, is recently reported. It is analogous to graphene, silicene, germanene and stanene in single-layered and hexagonal arrangement of atomic structure. In this paper, molecular dynamics simulations have been carried out to study the effect of sample size, temperature and strain velocity on the mechanical properties of plumbene. The results show superior mechanical properties of the single layer plumbene sheet which is several times higher than bulk lead making it a suitable candidate for using as reinforcement to develop high strength nanocomposites.

1. Introduction

Reduction in dimensionality of a material reduces the available phase space and diminishes screening which lead to enriched quantum effects and increased corrections. As a result these materials exhibit exceptional properties. Nanomaterials have wide range of potential applications due to enhanced mechanical, electrical, thermal, optical and chemical properties than bulk materials. [1–7] Graphene, the two-dimensional allotrope of carbon, due to its impressive mechanical and thermal [6–8] properties is widely used now-a-days in industries [9,10] where mechanical stability and thermal conductivity are the main concerns. Silicene, germanene and stanene also have promising properties for wide range of applications [11–13].

Plumbene [14–16] is a single layer of sp-hybridized lead atoms tightly packed into a two-dimensional hexagonal structure analogous to graphene and other members of the group. Pb-Pb bond distance in plumbene is 3 Å. This 2D nanomaterial has a large band gap of ~400 meV which is higher than other topological materials with band gap of ~200 meV [15]. Graphene have no band gap normally but a band gap of 2 meV can be induced in it by doping silicene as n-type dopant in graphene [17]. Silicene itself have a band gap of ~20 meV approx. Hence band gap of plumbene is even greater than graphene and silicene [18]. Like plumbene silicene is also more stable in buckled structure than planar structure and have the tendency to form sp^2 hybridization [19]. Silicon possesses higher band gap 1.25 to > 3 eV under different operational conditions than plumbene [20,21]. Germanene have interatomic distance and band gap of 4.061 Å and 0.06 eV [22,23]. By proximity coupling of graphene to antiferromagnetic material quantum anomalous Hall effect is realized in it and it also have stronger hybridization than plumbene (topological insulator) [24]. Quantum Anomalous Hall (QAH) effect is also observed in other hexagonal metal-oxide Nb_2O_3 which results its application as a topological insulator [25]. Similarly stanene, the honeycomb-like structures of tin atoms have strongest spin-orbit-coupling (SOC) effect for which the nontrivial topological insulator state can drive and stabilized by them. This also gives rise to new Quantum Spin Hall effect (QSH) insulators in stanene film [26,27]. QSH phenomenon is also noticed in functionalized Bi/Sb(1 1 1) films and thus they found application as a dissipationless transport device at room temperature [28]. But nanomaterials have many other advantages over bulk materials hence targeted to be used replacing conventional bulk materials. Zhao et al., also have predicted very high band gap of 1.03 eV to 1.34 eV in plumbene by

* Corresponding author.
E-mail address: gournetaidas@rocketmail.com (D.K. Das).

https://doi.org/10.1016/j.commatsci.2018.05.006
Received 31 December 2017; Received in revised form 10 April 2018; Accepted 4 May 2018

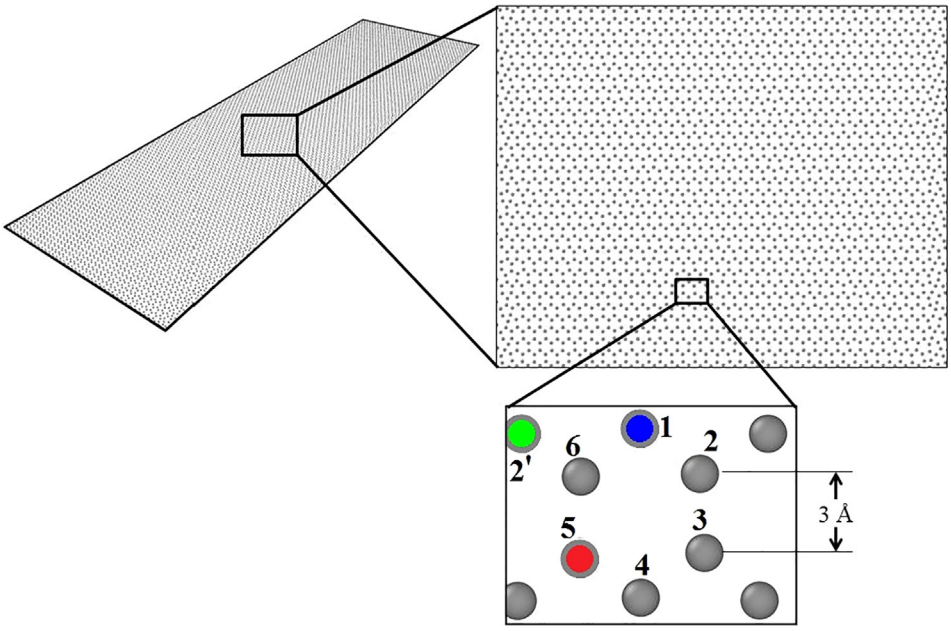

Fig. 1a. Our designed plumbene sheet (planar structure).

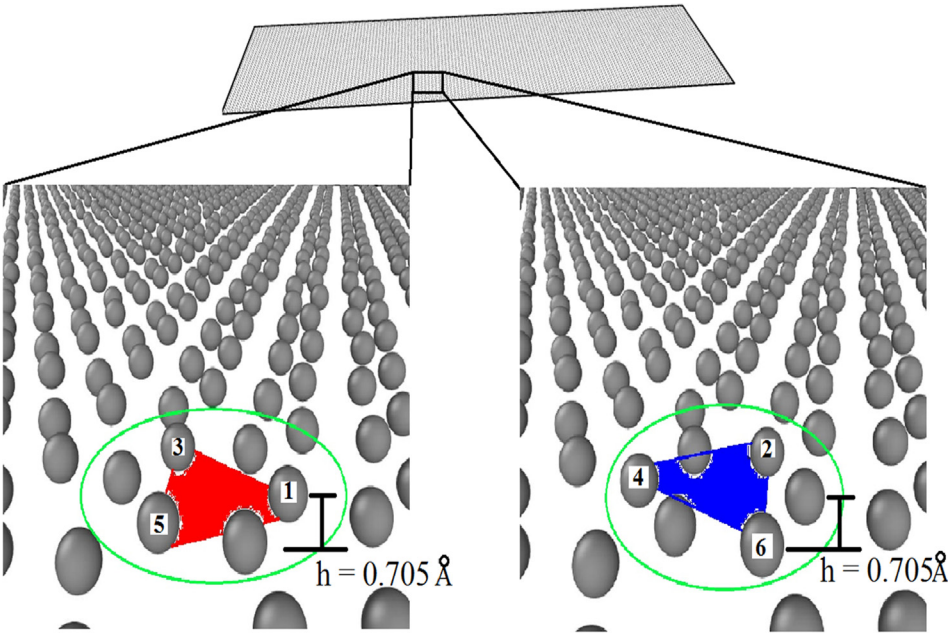

Fig. 1b. Our designed plumbene sheet (buckled structure).

doping different types of halides in it [16]. The buckling structure of plumbene enhances the overlap between σ and π orbitals. With increase in molecular weight of materials the type of hybridization changes from sp^2 to sp^3[14]. Plumbene is still a predicted material whose few properties like band gap, mechanism of hybridization among its bonds, structural symmetry are being calculated using first principal calculations and computational modeling. Experimental synthesis of plumbene is not reported till now. We have estimated the mechanical properties of plumbene using molecular dynamics simulations under tensile loading. The variation of mechanical properties of plumbene with variation in sample size, temperature, strain velocity and axis of loading are also reported here. The novelty of our work is earlier no such work of estimating mechanical properties of plumbene is reported. We found our estimated values of mechanical properties of plumbene like Young's modulus (E) and ultimate tensile strength (UTS) are much higher than bulk lead with E and UTS values 16 GPa and 12 to 17 MPa. Due to this band gap plumbene can found its applications as topological insulators and high temperature applications [15,16]. Plumbene with high