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Nanoindentation study of mechanical behavior and response of a single layer pristine silicene sheet using molecular dynamics simulations

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ABSTRACT

In the present study, molecular dynamics simulations were carried out to study the mechanical behavior and response of a single layer, rectangular, planar and pristine silicene sheet during nanoindentation process. The nanoindentation simulation on the silicene sheet was done using a spherical diamond indenter and the different force vs depth of indentation curves at different conditions of temperature, indenter radius and depth of indentation were obtained. The variation of mechanical properties like maximum force, hardness and Young's modulus were studied with respect to temperature, indenter radius and depth of indentation by varying one parameter while keeping the other two parameters constant. The deformation behavior of the silicene sheet up to failure was thoroughly studied and the mechanical properties like maximum force bearing capacity, maximum hardness and Young's modulus of the silicene sheet were calculated. The maximum force and hardness of the silicene sheet at its maximum indentation depth of 39.5 Å are found to be 286.3 nN and 461.2 GPa respectively. The Young's modulus of the silicene sheet is found to be 176.9 GPa which is in close agreement with the existing literature reported value of 178 GPa.

1. Introduction

Two dimensional materials show exceptional material properties owing to their densely packed, single layer, two dimensional hexagonal structures. Graphene [1] has emerged as the first two dimensional allotrope of carbon which shows excellent mechanical properties. The invention of silicene [2–4] – two dimensional, single layer, hexagonal allotrope of silicon, has drawn much attention among researchers due to its dense honeycomb crystal structure with mostly sp^3 hybridizations which gives rise to excellent material properties. Unlike graphene, silicene can exist both in planar as well as buckled form and the perfectly planar structure analogous to graphene is called silicene while the buckled form is called Si (1 1 1) sheet [4]. But silicene is predicted to be more stable in its buckled configuration which occurs due to pseudo John-Teller distortion effect having buckled length of 0.457 Å. Several researchers have widely studied and investigated the mechanical properties of different configurations of silicene [5–10]. Nanoindentation testing [11] is the most convenient and widely used process to determine material properties like hardness and Young's modulus of any material by applying load on the surface. A very rigid and hard material is used as indenter to slowly apply load on the surface then again unload from the surface and the variation of force with the depth of indentation is studied from the force vs indentation depth curve. The mechanical properties of the material like hardness and Young's modulus can be calculated from the force vs indentation depth data. Molecular dynamics prove to be a very convenient atomistic simulation tool which can be used to study the behavior of materials in atomic scale. Several researchers have studied the mechanical behavior of different materials by nanoindentation using molecular dynamics simulations [12–17]. Many researchers have also carried out simulations in molecular dynamics to widely study the mechanical response and material deformation behavior of two dimensional materials like single layer and multilayer graphene during nanoindentation [18–25]. But literature shows that no study has yet been reported on the mechanical behavior of single layer silicene sheet during nanoindentation.

So the novelty of this present work lies on the study of mechanical behavior and response of a single layer, rectangular and pristine silicene sheet with planar configuration and subjected to nanoindentation test using molecular dynamics simulation technique. A hard and rigid spherical diamond indenter was used to apply force on the silicene sheet and the indentation process was carried out at a very slow rate. The force vs indentation depth

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curves during both the loading and unloading processes were obtained and the mechanical properties like maximum force, hardness and Young's modulus were calculated. The variation of these mechanical properties with test temperature, indentation depth and indenter radius were also thoroughly studied by altering one of the parameters while keeping the other two parameters constant. The deformation behavior of the silicene sheet at maximum indentation depth up to rupture was also thoroughly studied.

2. Computational methods

The nanoindentation simulations of the single layer, planar and pristine silicene sheet were done using an open-source Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software package [26], and the atomistic simulation data were visualized using an open-source software package 'OVITO' [27]. A three dimensional simulation box was generated at first inside which a single layer planar silicene sheet of length 700 Å and width 400 Å and also a rigid spherical diamond indenter of radius 20 Å were created. These structures were created using the in-built crystal structure generating algorithm in LAMMPS. The designed silicene sheet and indenter contain 38,052 and 5909 atoms respectively. The silicene sheet is oriented such that (0 1 0) plane is parallel to the length of the cylinder and (1 0 0) plane is parallel to the width of the cylinder. The indenter was created in such a way that (0 0 1) plane is parallel to the axis of the indenter and the motion of the indenter is restricted along the [0 0 1] direction. The indenter was created and placed just at a certain distance above the exact center of the silicene sheet. Fig. 1(a) shows the generated silicene sheet and indenter and Fig. 1(b) shows the zigzag and armchair configuration in the silicene sheet denoted by red and blue color respectively. The zigzag configuration is oriented along the [1 0 0] direction while the armchair configuration is oriented along the [0 1 0] direction.

The generated sheet and indenter were assigned an initial velocity according to Maxwell-Boltzmann energy distribution function [28] that corresponds to their equilibration temperature and can be expressed as:

$$f_E(E) = \frac{n(E)dE}{N} = 2\sqrt{\frac{E}{\pi}}\left(\frac{1}{2kT}\right)^{\frac{3}{2}} \exp\left(-\frac{E}{kT}\right) \quad (1)$$

where, N number of atoms are considered to be present in our system, k is the Boltzmann's constant and $f_E(E)$ atoms have kinetic energy between E and $E + dE$. Periodic boundary conditions were considered along the x- and y-directions and non-periodic shrink-wrapped boundary along the z-direction. After the initialization of position and velocities of each atom, the indenter as well as the sheet were subjected to thermal equilibration and relaxation at a temperature of 300 K using a canonical NVT ensemble. Nosé-Hoover thermostat [29] was used for the time integration on non-Hamiltonian equations of motion which updates the position and velocity of a group of atoms with each timestep. The accuracy of a simulation depends totally on the choice of interatomic potential function which are used to define the interatomic interactions at the nanoscale. For covalent system with diamond cubic structure like C and Si, the effect of covalent bonds and bond angles should be taken into account which is best considered by the Tersoff [30] potential and it is expressed as:

$$E = \sum_i E_i = \frac{1}{2}\sum_{i \neq j} V_{ij} \quad (2)$$

where, E and V_{ij} are the total energy and bond energy of the atoms respectively. V_{ij} can be defined as the function of cut-off distance (f_C), repulsive pair potential (f_R) and attractive pair potential (f_A), which can be expressed as:

$$V_{ij} = f_C(r_{ij})\lfloor a_{ij} f_R(r_{ij}) + b_{ij} f_A(r_{ij})\rfloor \quad (3)$$

where,

$$f_C(r) = \begin{cases} 1 & : r < R - D \\ \frac{1}{2} - \frac{1}{2}\sin\left(\frac{\pi}{2}\frac{r-R}{D}\right) & : R - D < r < R + D \\ 0 & : r > R + D \end{cases}$$

$$f_R(r) = A\exp(-\lambda_1 r)$$

$$f_A(r) = -B\exp(-\lambda_2 r)$$

$$b_{ij} = \left(1 + \beta^n \zeta_{ij}^n\right)^{-\frac{1}{2n}}$$

$$\zeta_{ij} = \sum_{k \neq i,j} f_C(r_{ik}) g(\theta_{ijk}) \exp\left\lfloor \lambda_3^3 (r_{ij} - r_{ik})^3 \right\rfloor$$

$$g(\theta) = \left(1 + \frac{c^2}{d^2} - \frac{c^2}{\left[d^2 + (h - \cos\theta)^2\right]}\right)$$

Tersoff potential considered the individual interactions among the carbon atoms and the silicon atoms respectively. The cross-interaction between carbon and silicon atoms was modelled using a Morse potential [31] which computes pairwise interaction given by:

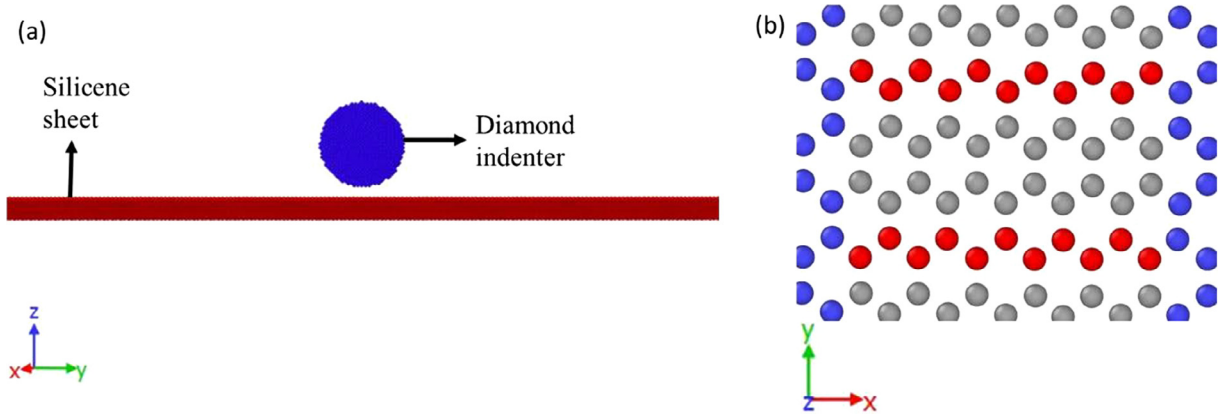

Fig. 1. (a) Silicene sheet and diamond indenter generated using LAMMPS and (b) zigzag (red) and armchair (blue) configuration of the silicene sheet. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)