



Fracture behavior of hydrogen-functionalized silicene nanosheets by molecular dynamics simulations



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ABSTRACT

Molecular dynamics simulations are used to investigate the mechanical properties of the hydrogen-functionalized silicene nanosheets (silicane). The nanosheet elastic modulus, fracture stress and strain are computed. It is shown that the mechanical properties of the silicene nanosheets degrade by functionalizing with hydrogen atoms. Comparing the mechanical properties of armchair and zigzag silicene and silicane nanosheets, it is shown that the armchair nanosheets have higher Young's modulus, fracture stress and fracture strains than the zigzag silicene and silicane nanosheets with the same dimensions. Following up the fracture pattern of the silicane nanosheets, a brittle behavior is observed for both of the armchair and zigzag nanosheets. It is also shown that the mechanical properties of the armchair and zigzag silicane has an inverse relation to the temperatures.

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1. Introduction

The fantastic properties of graphene [1–3] have led to motivating the research community to search for other 2D nanostructures with the same properties [4–12]. Specially, the group -IV monolayers have been considered by different researchers [13–17]. Silicene, a monolayer silicon (Si) nanosheet, is one of nanostructures that due to its current use in semiconductor electronics [18] combined with a similar carbon-like lattice, have been investigated extensively [19–31]. It has been successfully synthesized on silver [32,33,21,34–38], zirconium diboride [39] and Ir(111) [40] substrates. It has also recently been synthesized on tungsten diselenide [41], graphite [42] and h-MoS₂ [43]. Moreover, ion implantation has also been employed to synthesize the silicene nanosheets [44].

Several studies have been performed on the mechanical properties of the silicene [45–60]. The elastic and plastic deformation of silicene under uniaxial tension were investigated along with graphene, and boron nitride (BN) honeycomb nanoribbons by Topsakal and Ciraci [45]. They showed that the electronic structure of the silicene is strongly modified under the tensile loading. Besides, the in-plane Young's modulus of graphene was obtained as 62 N/m. Ince and Erkoç [46] used classical molecular dynamics (MD) simulations to study the structural properties of silicene nanoribbons (SiNRs) under 5% and 10% uniaxial strain. They showed that under strain, SiNRs have very ductile behavior with

a significant toughness and a very long plastic range before fragmentation. Comparing the configuration of the silicene nanoribbons under the tensile loadings, in 1 K and 300 K, less necking initiation points were observed in 300 K and hence, fragmentation occurs at larger strain.

The first-principles calculations was used by Qin et al. [47] to investigate the mechanical and electronic properties of silicene under strains. The yielding strain of silicene under uniform expansion was found about 20%. Besides, the in-plane Young's modulus of the armchair nanoribbon (10) was obtained as 51 J/m². Jiang et al. [48] computed Young's modulus of silicene by using ab initio calculation and MD simulations with different empirical potentials. It was shown that the critical strain and stress of bulk silicene under uniaxial tension are strongly dependent on the nanosheet chirality. The elastic modulus of the armchair and zigzag bulk silicene were computed as 140.7 GPa and 148.5 GPa, respectively. Comparing the results of MD simulations by four different force-fields, including EDIP, Erhart-Albe, SW and MEAM with the ab initio simulations, they concluded that the first force field can leads to more accurate results than the other models.

Using density functional theory (DFT), the mechanical stabilities of planar (g) and low-buckled (b) honeycomb monolayer structures of silicon under various large strains were investigated by Peng et al. [49]. They showed that increasing pressure leads to increasing the second order elastic constants, including in-plane stiffness. However, Poisson's ratio decreases by increasing the pressure. They found the in-plane elastic modulus of the g-Si and b-Si as 71.2 N/m and 63.8 N/m, respectively. Besides, correspond-

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ing Poisson's ratio were computed as 0.401 and 0.325, respectively. Xu et al. [50] used first-principles calculations to investigate the atomic structures and nonlinear properties of single layer graphene (SLG), bilayer graphene (BLG), single layer silicene (SLS), and bilayer silicene (BLS) under equiaxial tension and uniaxial tensions. The in-plane elastic modulus of the SLG, BLG, SLS and BLG were obtained as 334.77 GPa, 419.77 GPa, 63.3 GPa and 68.25 GPa, respectively. In other words, the BLG and BLS possess a slightly larger in-plane stiffnesses than their single layer counterparts.

Using first principle calculations, Qin et al. [51] investigated the mechanical and electronic properties of the silicene nanosheet under the uniaxial loading. They indicated that Poisson's ratio and the rigidity of silicene are strongly dependent on its chirality. Using MD simulations, Ansari et al. [52] represented that the ultimate strain of armchair silicene is larger than that of graphene. However, the zigzag graphene has a larger fracture strain than the zigzag silicene. They also represented that the stiffness of silicene is about one-fourth of the stiffness of the graphene with the same dimensions. Utilizing DFT calculations, Wang et al. [53] studied the behavior of silicene under tensile strain. It was indicated that the buckled single-layer silicene transits to planar hexagonal silicene at a critical tensile strain of 0.20. Moreover, they observed a strong anisotropy in Poisson's ratio of the silicene.

Employing MD simulations, Roman et al. [54] investigated the mechanical properties of the armchair and zigzag silicene. They showed that the bending rigidity of silicene is 38.63 eV which falls between the bending rigidity of single-layer (2.1 eV) and bi-layer graphene (130 eV).

The distributions, unbuckling mechanisms and the fracture dependence of silicene on the temperature were discussed by Botari et al. [55] by MD simulations. It was represented that the fracture strain and fracture stress of the silicene depend on the temperature, significantly. Moreover, they claimed that Young's modulus of the silicene is isotropic. However, anisotropic behavior was observed in the critical strain. The effects of temperature and strain rate on the mechanical properties of silicene were explored by Pei et al. [56] by using the MD simulations. They showed that the fracture strength and fracture strain of silicene experience significant reduction by increasing the temperature. However, the effect of strain-rate on the silicene mechanical properties is negligible. The MD simulations was used by Chavez-Castillo et al. [57] to study the dependence of Young's modulus of silicene to size, vacancy defect and temperature. It was found that Young's modulus of defect-free and defective silicene are function of length and temperature.

The roles of vacancy and SW defects on the mechanical properties of silicene were studied by Le and Nguyen [58]. They showed that the elastic properties of the silicene nanosheet are not significantly affected by the existence of the small amount of the defect. However, the single defect can decrease the fracture strength and fracture strain, significantly. For example, removing only two atoms from the center of the silicene can leads to 18–20% reduction in fracture stress and 33–35% in fracture strain. The mechanical properties of the silicene nanosheets with edge cracks were studied by Yuan et al. [59] with the aid of MD simulations. They showed that the critical strain and fracture stress of the armchair silicene degrades significantly by introducing the edge crack.

The first-principles calculations were also used to investigate the fully oxidized silicene and germanene [60]. They observed a significant anisotropy in the mechanical and electrical properties of the fully oxidized silicene and germanene. It was also shown that the considered structures have prominent elastic characteristics with a negative Poisson ratio. It has been proved that complete hydrogenation can lead to modification of the electronic properties of the silicene [61]. Therefore, the electronic [61–68] and mechan-

ical [68,69] properties of the hydrogenated silicene so-called silicane, have been investigated by different researchers. Using first principle calculations, Zhao [68] investigated the effect of strain and chirality on the mechanical and electronic properties of silicane. He indicated that the elastic modulus of the silicene decreases by fully hydrogenation. Peng and De [69] also used DFT simulations to investigate the elastic properties of silicane. They obtained the elastic limit of the silicane as 0.22, 0.28, and 0.25 along armchair, zigzag, and biaxial directions, respectively. Besides, Poisson's ratio of silicene was obtained as 0.240.

Although the mechanical properties of the silicene has been extensively investigated, no comprehensive work can be found on the mechanical properties of silicane by MD simulations. In this paper, MD simulations are performed to investigate the mechanical properties of the silicane nanosheets. The elastic modulus, fracture strain and fracture strain of the silicane nanosheets are compared with those of the silicene nanosheet. Besides, the effects of the geometrical parameters of the silicane nanosheets on its mechanical properties are evaluated. The mechanical properties of the armchair and zigzag silicane is also investigated at different temperatures. Finally, to investigate effect of boundary H atoms on the properties of the silicane, the stress-strain curves of the nanosheets with and without boundary H atoms are compared.

2. Details of MD simulations

Mechanical properties of the silicane nanosheet are evaluated by MD simulations here. The geometrical parameters of the simu-

Table 1
Geometrical parameters of simulated nanosheets [68].

Geometrical parameter	Silicene	Silicane
$d(\text{\AA})$	2.28	2.36
$\theta(\text{degrees})$	116.25	111.09
$\delta(\text{\AA})$	0.45	0.72
$d_H(\text{\AA})$	–	1.50

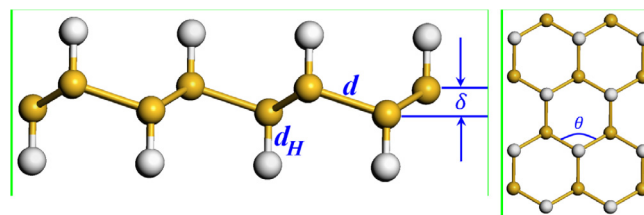


Fig. 1. Schematics of the geometrical parameters of simulated nanosheets.

Table 2
The employed parameters in the interatomic potentials.

Parameter	Si-Si [74]	Si-H [75]	H-H [76]
$A(\text{eV})$	1830.8	323.54	80.07
$B(\text{eV})$	471.18	84.18	31.38
$\lambda_1(\text{\AA}^{-1})$	2.4799	2.9595	4.2075
$\lambda_2(\text{\AA}^{-1})$	1.7322	1.6158	1.7956
$\alpha(\text{\AA}^{-1})$	5.1975	4.00	3
β	3	3	1
$R^{(e)}(\text{\AA})$	2.35	1.475	0.74
c	—	0.0216	4.00
d	0.160	0.27	—
h	-0.59826	-1.00	-1.00
$R(\text{\AA})$	2.85	1.85	1.40
$D(\text{\AA})$	0.15	0.15	0.30
η	0.78734	1.00	1.00
δ	0.635	0.80469	0.80469

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