Understanding mechanical properties and failure mechanism of germanium-silicon alloy at nanoscale

Md. Habibur Rahman · Emdadul Haque Chowdhury · Md Mahbubul Islam

Abstract We use molecular dynamics simulations to investigate the material properties of cubic zinc blende Si$_{0.5}$Ge$_{0.5}$ alloy nanowire (NW). We elucidate the effect of nanowire size, crystal orientations, and temperature on the material properties. We found that the reduction in the NW cross-sectional area results in lower ultimate tensile strength (UTS) and Young’s modulus. The [111] and [110] oriented NWs exhibit the highest fracture strength and fracture toughness, respectively. The increased temperature degrades the strength of the material and facilitates failure. The vacancy defects introduced via removal of either Si or Ge atoms exhibit similar behavior, and linear reduction of UTS and Young’s modulus are realized with an increased vacancy concentration. We observed intrinsic failure characteristics of the NW as insensitive to the temperature. Overall, the new understanding of material properties and failure characteristics of Si$_{0.5}$Ge$_{0.5}$ NW elicited in this study will be a guide for designing Si–Ge-based nanodevices.

Keywords Silicon-germanium · Molecular dynamics · Tersoff potential · Nanodevices · Thermoelectric · Nanostructures

Introduction

Silicon-germanium (Si$_x$Ge$_{1-x}$) is an alloy with any molar ratio of silicon (Si) and germanium (Ge). Si$_x$Ge$_{1-x}$ is a semiconducting and thermoelectric material that has been successfully deployed in heterojunction bipolar transistor, strained metal-oxide-semiconductor (MOS), complementary metal-oxide-semiconductor (CMOS), and many other electronic systems (Haddara et al. 2017; Wang et al. 1995). Recently, nanowires (NW) have received significant attention in the scientific community for their distinctive thermal, mechanical, electronic, and optical properties and extensively studied for potential applications as building blocks in nanoelectromechanical devices (NEMS) (Lu and Lieber 2006; Hochbaum and Yang 2010; Rurali 2010). The NWs are excellent candidates for optoelectronic and nanoelectronics devices (Zhang et al. 2011), detectors, and sensors for biological and chemical applications (Eom et al. 2011), ultrahigh-frequency resonators (Feng et al. 2007), and energy harvesting (Lee et al. 2012).

The Si NWs are extensively studied because of their exceptional properties and enormous applications in electrical and optical nanodevices and NEMS (Morales and Lieber 1998; Cui and Lieber 2001; Cui et al. 2001; 2003). The mechanical deformation behavior and fracture mechanisms of Si NWs are probed using various
experimental analysis of Si$_x$Ge$_{1-x}$ alloys at an empirical or at the atomic scale. Several theoretical studies have been conducted to perform local structural analysis of Si$_x$Ge$_{1-x}$ nanowire employing first-principle calculations. Likewise, investigations in Ge NWs revealed interesting properties. Smith et al. (2008) found that Young’s modulus remains independent of change in NW diameter for a range of 50 to 140 nm sample size, while Wu et al. (2008) reported extraordinary mechanical strength for Ge nanowire and thus ability to store elastic potential energy. Mingo et al. (2003) investigated the mechanical and thermal properties of the Si and Ge nanostructures.

Silicon-germanium alloys are of great interest for a wide variety of applications, such as high-mobility transistors and thermoelectric devices (Vining et al. 1991; Vining 1991). The Si–Ge alloys are a perfect model system to analyze the possibilities and limitations of atomic-scale simulation. Ge and Si both possess a ground-state diamond-lattice structure (Stampfl and Bennemann 1990; Paulus et al. 1995). Several theoretical studies have been conducted to perform local structural analysis of Si$_x$Ge$_{1-x}$ alloys at an empirical or at the semi-empirical level. The structures have been found experimentally and with simulation (Weakliem and Carter 1992) as truly random, with no considerable long- or short-range compositional ordering. The thermal resistivity of Si–Ge alloy was inspected with molecular dynamics (MD) simulation by Skye and Schelling (2008). A combined electronic-structure and statistical-mechanical approach were adopted to disclose the thermodynamic properties of Si$_x$Ge$_{1-x}$ alloys by Qteish and Resta (1988). Georgakaki et al. (2014) performed MD simulations to investigate the vibrational and mechanical properties of clamped-clamped rectangular Si$_x$Ge$_{1-x}$ and Si–Si$_x$Ge$_{1-x}$ nanowires (NWs). They investigated the beat vibration phenomenon, the frequency response, and determined the mechanical properties such as quality factor and Young’s modulus. A contemporary work by Ma et al. (Ma et al. 2013) reported the tuning of Si–Ge alloy superlattice mechanical properties by changing the composition of Ge. Meanwhile, Kim et al. (2006) examined the size effect on Young’s modulus of Si–Ge alloy using MD simulations. Amato et al. (2014) recently presented an analysis covering a wide range of applications of Si–Ge nanowires. Furthermore, lattice defects are inevitable in nanomaterials during growth and processing. The physical processes such as stress, sublimation, and irradiation can also lead to a substantial concentration of such defects (Li and Zhang 2012). Vacancy defects are lattice sites which, in a perfect crystal, would be occupied but instead remain vacant. Along with a significant influence on mechanical properties (Fang and Zhang 2011), they also cause localization of lattice vibration around the defects.

Despite the efforts put forth to understand the properties of the Si–Ge alloys, the issues such as the effect of temperature, cross-sectional area, various defects, and crystal orientation on the tensile mechanical properties and failure mechanisms of NWs remain elusive. To the best of our knowledge, although there are several studies for the inspection of Si–Ge nanowire as potential thermoelectric (Lee et al. 2012) or electronic devices (Ma et al. 2013), a comprehensive study for the mechanical properties of Si$_{0.5}$Ge$_{0.5}$ alloy and its failure mechanism has not been reported yet. Therefore, the current work aims to investigate the mechanical properties such as ultimate tensile strength (UTS), Young’s modulus of the Si$_{0.5}$Ge$_{0.5}$ alloy by changing various parameters such as temperature, cross-sectional area, loading direction, and the concentration of vacancy defects using MD simulations. To understand the effect of vacancy defect on Si$_{0.5}$Ge$_{0.5}$ alloy, vacancies are created by removing Si and Ge atoms randomly from the alloy matrix and corresponding mechanical properties are recorded for in-depth analysis. Finally, the failure mechanism of Si$_{0.5}$Ge$_{0.5}$ NW at 100 K and 600 K temperatures has been elucidated as well.

**Computational method**

We used molecular dynamics (MD) simulations using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) (Plimpton 1993) package for calculating the tensile properties of Si$_{0.5}$Ge$_{0.5}$ alloy. We employed Tersoff potential (Tersoff 1990) to describe the interatomic interactions between Ge–Ge, Si–Si, and Si–Ge atoms in the MD simulations. OVITO (Stukowski 2009) is used for all the atomistic visualizations. To investigate the effect of size on the tensile strength of the alloy, the cross-sectional area of the nanostructure is varied from 11.05 to 19.65 nm$^2$ by
maintaining a length to width ratio of 8:1 (Munshi et al. 2019; Pial et al. 2018). Three different crystal orientations are chosen that are [100], [110], and [111] to examine the directional dependency on the material properties of the alloy. Periodic boundary conditions are applied along the loading direction (X), while other directions are kept free (i.e., the surfaces of the NWs were exposed to vacuum) (Munshi et al. 2019). The equations of motion were integrated using the velocity Verlet algorithm (Munshi et al. 2019) with a time step of 1 fs. At first, the energy of the system is minimized using the conjugate gradient minimization scheme (Munshi et al. 2019). Before applying the tensile load, NVE (constant volume and energy) and NPT (constant pressure and temperature) equilibrations are carried out for 20 ps each followed by an NVT (constant volume and temperature) ensemble simulation of 10 ps. Afterward, a uniaxial tensile strain is applied along the loading direction at a constant strain rate of \(10^9 \text{ s}^{-1}\) under NVT ensembles to control temperature fluctuations. We acknowledge that the employed strain rate is significantly higher than the case of typical experiments; however, such high rates are routinely used in MD simulations to study the materials’ behavior within a reasonable simulation time with moderate computational resources (Munshi et al. 2019; Pial et al. 2018; Wang et al. 2013). The atomic stresses in our simulations are calculated using virial stress theorem, (Munshi et al. 2019; Pial et al. 2018) which stands as,

\[
\sigma_{\text{virial}}(r) = \frac{1}{\Omega} \sum_i \left( -\dot{m}_i \ddot{u}_i \otimes \ddot{u}_i + \frac{1}{2} \sum_{j \neq i} r_{ij} \otimes f_{ij} \right)
\]

In this expression, \(\Omega\) denotes the total volume of the nanowire, \(\dot{m}_i\) presents the mass of atom \(i\), \(\otimes\) is the cross product, \(\ddot{u}_i\) is the velocity component of atom \(i\), \(r_{ij}\) represents the distance between atom \(i\) and \(j\), and \(f_{ij}\) is the interatomic force exerted by atom \(j\) on atom \(i\) (Fig. 1).

To validate our computational approach and the interatomic potential parameters, we calculated the lattice constant of Si\(_{0.5}\)Ge\(_{0.5}\) and Young’s modulus (YM) of [100]-directed alloy NW with a cross-sectional area of 15 nm\(^2\) at 300 K and compared them with published literature (Skye and Schelling 2008; Georgakaki et al. 2014). The comparisons are presented in Table 1; one can see that our calculated data are in good agreement with the reference values. To the best of authors’ knowledge, the mechanical properties (e.g., elastic constant, YM) of Si–Ge alloy NW have not been reported experimentally. Previously, Levinshtein et al. (2001) developed an empirical relation to predicting the bulk YM of Si–Ge binary eutectic system which is \(Y_0 = 130.2 - 28.1x\), where \(Y_0\) denotes the YM of bulk Si\(_x\)Ge\(_{1-x}\) alloy

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Fig. 1 a Initial coordinates of 31.60 nm × 3.92 nm × 3.92 nm Si\(_{0.5}\)Ge\(_{0.5}\) alloy NW. b Crystal structure of cubic zinc blende Si\(_{0.5}\)Ge\(_{0.5}\) alloy NW with a lattice constant of 0.554 nm
A system and $x$ denotes the composition of Ge. Using this empirical relation, we found YM of Si$_{0.5}$Ge$_{0.5}$ as ~ 116 GPa which nicely agrees with our MD simulation.

The excellent agreement between our simulation predictions and literature data indicates that the potential used in this study is well capable of describing the atomic interactions considered in this study. These observations motivate us to further investigate the tensile mechanical properties as well as the detailed failure behavior of the Si–Ge alloys.

**Results and discussions**

**Mechanical properties of pure Ge, pure Si, and Si$_{0.5}$Ge$_{0.5}$ alloy NW at 300 K** We perform an in-depth comparison of the stress-strain response and mechanical properties of pure Si, pure Ge, and the Si$_{0.5}$Ge$_{0.5}$ alloy NW at 300 K.

The characteristic stress-strain profiles of pure Ge, pure Si, and Si$_{0.5}$Ge$_{0.5}$ alloy NWs for [100] loading direction at 300 K are illustrated in Fig. 2. It is evident from the figure that all the three NWs manifest a typical brittle type fracture. YM is obtained by calculating the slope of the initial elastic portion of the stress-strain curves (up to 4% of strain), which are documented in Table 2 along with fracture stresses and strains. Si NW is ascertained to have the maximum fracture stress and fracture strain values, while they are the lowest for the Ge NW. Our MD simulation results suggest that the UTS and the fracture strain of Si$_{0.5}$Ge$_{0.5}$ NW lie in between pure Si NW and pure Ge NW. This phenomenon can be ascribed to the difference in interatomic bond strength of these NWs. The relatively smaller interatomic distance between Si–Si atoms in the Si NW contributes to a relatively greater bond strength than the Ge–Ge bonds, which inherit a larger interatomic bond length. Note that the bond length and the bond strength of Si–Si bonds are 233 pm and 222 kJ/mol, respectively (Huheey and Cottrell 1958), while the bond length and the bond strength of Ge–Ge bonds are 241 pm and 188 kJ/mol, respectively (Huheey and Cottrell 1958). Consequently, it requires a high fracture strain and corresponding fracture strength to break the Si–Si bonds compared with the Ge–Ge bonds, rendering Si–Si bonds difficult to deform and harder to break. In the case of Si$_{0.5}$Ge$_{0.5}$ alloy NW, a considerable amount of Ge–Ge bond is present in the alloy, resulting in a lower value of UTS, fracture strain, and YM of the Si$_{0.5}$Ge$_{0.5}$ alloy compared with pure Si NW. Next, we carried out MD simulations to explore the effects of NW size, temperature, loading direction, defects on the tensile strength, as well as temperature-dependent fracture process of the Si$_{0.5}$Ge$_{0.5}$ alloy NW.

**Size and temperature-dependent mechanical properties of the [100]-oriented Si$_{0.5}$Ge$_{0.5}$ NW** We comprehensively characterize the combined impacts of temperature and NW size on the uniaxial tensile mechanical attributes of the [100]-directed Si$_{0.5}$Ge$_{0.5}$ alloy NW. The stress-strain response of Si$_{0.5}$Ge$_{0.5}$ alloy with a 15-nm$^2$ cross-section under tension for 100–600 K is shown in Fig. 3a. From the stress-strain diagram, it is apparent

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**Table 1** Comparisons of calculated properties and literature data

| Property                                      | This study | Literature               |
|-----------------------------------------------|------------|--------------------------|
| Lattice parameter of Si$_{0.5}$Ge$_{0.5}$ alloy | ~ 0.557 nm | ~ 0.545 nm (Skye and Schelling 2008) |
| YM of Si$_{0.5}$Ge$_{0.5}$ alloy NW            | ~ 91.89 GPa| ~ 86 GPa (Georgakaki et al. 2014) |
| YM of Bulk Si$_{0.5}$Ge$_{0.5}$ alloy          | ~ 126 GPa  | ~ 116 GPa (Levinshtein et al. 2001) |

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**Fig. 2** Stress-strain response of [100]-oriented pure Ge, pure Si, and Si$_{0.5}$Ge$_{0.5}$ alloy at 300 K
that up to a certain point (4% strain), stress increases linearly with increasing strain; thus, material exhibits elastic behavior in that region (Munshi et al. 2019; Pial et al. 2018). Thereafter, stress increases non-linearly until it reaches the UTS succeeded by an abrupt decrease with a small increase in strain (Munshi et al. 2019; Pial et al. 2018). The sudden decrease in stress indicates a brittle-type failure of the alloy. At 100 K, the UTS is calculated as ~ 18.6 GPa, with a corresponding failure strain of ~ 35%. As the temperature increased from 100 to 600 K, the UTS of the alloy reduced to ~ 14.21 GPa, with a much lower fracture strain of ~ 22.23%. Consequently, the fracture toughness viz., the total energy absorbed before fracture, evaluated from the area under the stress-strain curve, monotonically decreases with increasing temperature. These behaviors can be attributed to the temperature-induced weakening of the chemical bonds in the crystal owing to enhanced atomic mobility and increased mean interatomic distance at elevated temperatures. To observe the effects of size on the uniaxial tensile behavior of the Si0.5Ge0.5 alloy at the nanoscale, three different cross-sectional areas are chosen that are 11.05 nm², 15.00 nm², and 19.65 nm². The corresponding simulation results at 300 K are plotted in Fig. 3b. It is apparent from this figure that the stress-strain response depends on the cross-sectional area of the alloy at the nanoscale, although material properties such as UTS and YM are independent of material geometry at the bulk level. Therefore, we can conclude that the analysis of continuum mechanics may not be appropriate to determine material properties at the nanoscale. Such observed characteristics of nanomaterials that are different from their bulk counterparts have been reported in previous literature as well (Smith et al. 2010; Pearson et al. 1957; Hanrath and Korgel 2004). The difference in the properties can be primarily attributed to the de-cohesion effect (Liang et al. 2005; Huang et al. 2011) of the surface atoms as the NW contains a large percentage of surface atoms owing to the increased surface-to-volume ratio at the nanoscale.

The variations of UTS and YM as a function of temperature for different cross-sectional areas are presented in Fig. 3c, d. The YM is obtained by evaluating the slope of the stress-strain curve within the elastic limit (strain values < 4%) (Munshi et al. 2019; Pial et al. 2018). It can be observed that there is a significant impact of size on the mechanical properties of Si0.5Ge0.5 alloy, while it undergoes [100] loading direction. Both UTS and YM manifest a strong inverse relationship with temperature for all cross-sectional areas; nevertheless, they are observed to increase with increased cross-sections. Such enhancement in tensile properties of the Si0.5Ge0.5 NW with an increased cross-sectional area gives credit to the reduction in the surface-to-volume ratio of the material (Wang et al. 2013). The surface atoms are reported to play a crucial role in dictating the mechanical behaviors of nanomaterials since lattice defects are most likely to occur on the surface of nanostructures (Wang et al. 2013). Therefore, Si0.5Ge0.5 alloy having smaller cross-sections possesses a larger specific surface area, and thereby facilitates a higher percentage of lattice defects compared with the ones with greater cross-sections. The degree of lattice defects in the structure directly affects its UTS, fracture strain, and YM. Similar increment in UTS and YM with increased size was also found for other NWs such as Si (Lee and Rudd 2007; Zhu et al. 2009), SiC (Tsuuzuki et al. 2011), InP and InAs (Dos Santos and Piquini 2010), GaN (Shi-Feng et al. 2011), CdTe (Munshi et al. 2019), and Ni (Wang et al. 2013) NWs. For a case study, we also simulated the tensile properties of Si0.25Ge0.75 alloy NW which is presented in the supplementary information of this article (Fig. S1).

**Effect of crystal orientation on the mechanical properties of Si0.5Ge0.5 NW** We thoroughly analyze the effect of crystallographic orientation on the mechanical properties of Si0.5Ge0.5 alloy NWs. Figure 4a displays the typical stress-strain relations of Si0.5Ge0.5 alloys at 300 K temperature considering [100], [110], and [111] crystal orientations. It can be seen from the figure that the [111]-oriented Si0.5Ge0.5 alloy exhibits the highest UTS, followed by [110] and [100] orientations. This observation can be ascribed to the disparity of surface energy of the material along three crystal directions. As reported earlier, the [111] direction inherits the lowest surface energy among these three crystal orientations.

### Table 2 Comparison of mechanical properties of pure Ge, pure Si, and Si0.5Ge0.5 alloy NW at 300 K obtained in the present study

| Property           | Pure Ge NW | Pure Si NW | Si0.5Ge0.5 alloy NW |
|--------------------|------------|------------|---------------------|
| Young’s modulus (GPa) | ~ 84       | ~ 94       | ~ 91.89             |
| Fracture stress (GPa)   | ~ 12.03    | ~ 20.2     | ~ 16.11             |
| Fracture strain (%)     | ~ 22.2     | ~ 28.60    | ~ 25.8              |
because of the highest surface atomic distance, and hence the least density of surface atoms (Bin et al. 2014; Zhang et al. 2003; Lu et al. 2011). This relatively lower surface energy of [111] orientation renders it the most stable structure, thus enabling it to exhibit the highest resistivity against fracturing, and henceforth [110] and [100] orientations (Bin et al. 2014; Zhang et al. 2003; Lu et al. 2011). Such orientation-dependent mechanical properties were also reported for other NWs, including CdTe, W, and Si (Munshi et al. 2019; Bin et al. 2014; Kang and Cai 2010). Note that in reference (Munshi et al. 2019), for brittle CdTe semiconducting NW, authors reported plasticity for compressive loading while for tensile loading, they did not find any plasticity or noticeable dislocation motion, which is in line with our results. Nevertheless, the [110]-oriented Si$_{0.5}$Ge$_{0.5}$ alloy shows higher fracture strain compared with the other two crystal orientations. The area under the stress-strain curves, i.e., the fracture toughness, indicates that it is the largest for [110] orientation and the lowest for [100] orientation. To further unravel the effects of crystal directions on the mechanical properties of the alloy, Fig. 4b, c manifests the variations of the UTS and YM for different crystal orientations as a function of temperature.

Fig. 3  Stress-strain response of a [100]-oriented Si$_{0.5}$Ge$_{0.5}$ alloy of 15-nm$^2$ cross-sectional areas for different temperature, b Si$_{0.5}$Ge$_{0.5}$ NWs for the different cross-sectional areas at T = 300 K; variations of c ultimate tensile stress for different cross-sectional areas of Si$_{0.5}$Ge$_{0.5}$ alloy with temperature and d Young’s modulus for the different cross-sectional area of Si$_{0.5}$Ge$_{0.5}$ alloy with temperature
From Fig. 4b, it is evident that the rate of diminution of UTS with temperature is the highest and lowest for [111] and [100] orientations, respectively. Although the [111] orientation has the highest UTS in the overall temperature regime, interestingly, in the temperature range of 100 to 200 K, [110] orientation provides slightly better performance than [111] direction in terms of YM (Fig. 4c). This might be derived from the fact that, in the ZB system, the interplanar distance along [110] direction is a little smaller than that of [111] direction (Munshi et al. 2019). Thus, at low temperatures, the interatomic bonds become slightly stronger between {110} planes, which contributes to marginally improved elasticity of the atomic links. Nevertheless, as the temperature rises, the role of this interatomic distance loses its prominence owing to enhanced atomic mobility. Therefore, when a tensile load is applied in [110] direction, due to the atomic arrangements in the crystal plane, fast accumulation of stress occurs at relatively lower temperatures which lead to a higher YM compared with [111] crystallographic direction. It can be also observed that the YM in [100] crystallographic direction is quite independent of temperature. Previously, it is reported that the surface of semiconductor materials tends to undergo reconstruction and surface energy of the reconstructed surfaces are found to be quite similar for different crystal orientation (Stekolnikov et al. 2002). However, in our MD simulation, surface reconstruction is not taken into consideration; rather, we confirm that different surfaces for different crystal orientations are terminated identically. Additional information can be found in the supplementary information of this article (Fig. S2).

**Effect of vacancy defects on the mechanical properties of Si$_{0.5}$Ge$_{0.5}$ alloy NW**

According to Griffith’s theory, the shape and size of defects play a more significant role than the bonding strength in determining the fracture strength (Lajtai 1971). Among various types of defects, the vacancy defect has a marked impact to govern the tensile properties of materials (Sun et al. 2014). More specifically, inducing only 2% of randomly dispersed mono-vacancies can deteriorate the fracture strength by $\sim 40\%$ in graphene (Sha et al. 2016). In this study, we only considered the effect of randomly distributed mono-vacancies, introduced via removal of Si and Ge atoms from the alloy, on the materials’ strength. The variation of uniaxial tensile mechanical properties of the Si$_{0.5}$Ge$_{0.5}$ as a function of Si and Ge vacancy concentrations is illustrated in Fig. 5, respectively, at 300 K. The impact of these defects arises from the under coordinated atoms and formation of dangling bonds around the random vacancies of the structure (Shi-Feng et al. 2011). From Fig. 5a, it is evident that as the percentage of monoatomic Si-vacancy defects increases, the value of UTS decreases continuously. These results are more profoundly illustrated in Fig. 5b, c. Both UTS and YM decrease almost linearly with increased concentration of vacancy defects. Introducing only 5% vacancy causes a reduction in the fracture strength and YM of about 14.21% and 11.15%, respectively, and similar behavioral change was reported for GaN NW as well (Shi-Feng et al. 2011). These dramatic degradations in the tensile properties can be attributed to the randomly missing atoms disrupting the integrity of the equilibrium stress field. The random removal of some atoms and the associated atomic linkages results in the formation of
some weak and dangling bonds around the defected region (Shi-Feng et al. 2011). Under such large variation in mass and strain, these spots near vacancy defects serve as a nucleation site for massive stress concentration under tension. Consequently, both chemical instabilities and mechanical nonequilibrium arise in the stretched alloy matrix (Jing et al. 2012). This accumulation of stress around vacancies facilitates the destruction of bonds between nearby members and eventually, the formation of the initial crack (Sun et al. 2014). Therefore, the bonds at the defect region can break much earlier in the course of the deformation process, allowing the structure to fail at a lower strain.

The effects of the removal of some random Ge atoms from the Si$_{0.5}$Ge$_{0.5}$ alloy are elucidated in Fig. 5d–f. Interestingly, the stress-strain profiles, UTS, and YM exhibit fairly similar responses irrespective of the type of atom extracted. Hence, it can be inferred that the UTS and the YM of the alloy are almost independent of the type of atoms eliminated from the structure. This gives credit to the fact that the vacancy defects primarily facilitate the initial crack nucleation and structural yielding. The subsequent deformation stages and the ultimate failure depend entirely on the atomic configuration of the system and crack propagation mechanism. Therefore, the type of atoms removed mainly contributes to initiating the fracture process. As the composition of the rest of the structure is essentially the same, it takes nearly the same amount of energy for complete rupture.

**Failure characteristic of Si$_{0.5}$Ge$_{0.5}$ NW** The failure behavior of Si$_{0.5}$Ge$_{0.5}$ alloy corresponding to different strain values at 100 K and 600 K is elucidated in Fig. 6. The process of fracture is profoundly dependent on the mechanism of crack propagation. In the case of ductile material, extensive plastic deformation typically takes place ahead of the crack tip, and consequently, ductile materials fail to owe to this plastic deformation. Once the applied load surpasses the UTS, the cross-section can no longer endure the applied load, which leads to necking and eventual failure of the material (Callister and Rethwisch 2018). Nonetheless, such plastic deformation is usually absent ahead of the crack tip in
the case of brittle materials. In the location of cracks, there is a massive accumulation of stress, culminating in an instantaneous fracture of the material owing to rapid crack propagation (Callister and Rethwisch 2018). The crack often propagates via cleavage of atomic bonds along specific crystallographic planes (cleavage planes), where shear stress becomes maximum (Callister and Rethwisch 2018; Wang et al. 2008; 2010).

At 100 K temperature (Fig. 6a), prior to 34.18% applied strain, no structural defects appear in the alloy. At 34.18% strain, crack nucleation and primary displacement of atoms start to occur. Upon further stretching, the rapid crack propagation continues nearly perpendicular to the direction of applied strain and the effective cross-sectional area continuously reduces. When the strain reaches 34.33%, an interesting phenomenon occurs. At this point, the cross-section eventually resembles the form of a neck, like a ductile material. An enlarged view of necking is provided in the supplementary information of this article (Fig. S3). In this scenario, brittle fracture takes place before any dislocation moves across the specimen. Also, no clean cleavage cut (no smooth surface after fracture) is observed, but instead, the material failed with a gradual decrease in cross-section and neck formation. At 600 K temperature (Fig. 6b), as the bond strength between Si–Si, Si–Ge, and Ge–Ge decreases, deformation in the alloy is found at 22.15% strain which is significantly earlier than 100 K temperature. The formation of the neck commences with only around 22.26% strain. At approximately 22.40% of strain, the structure can be attributed to a near failure condition that is 34.84% earlier than 100 K temperature. It is worth mentioning that, despite the alloy being a brittle material, the fracture process ends with the development of a neck that is the characteristic of ductile material failure. However, note that, in ductile material, the failure process proceeds relatively slowly as the crack length extends. A relatively prolonged period, and thus, a large range of strain are required for the material to undergo the step-by-step failure processes that are necking, cavity formation, cavity coalescence to form an elliptical crack, crack propagation, and ultimate fracture (Wang et al. 2013; Bin et al. 2014; Callister and Rethwisch 2018). However, in the case of Si_{0.5}Ge_{0.5} alloy, neck formation and eventual fracture occur very rapidly. Another difference in the failure processes between these two temperatures is that, at 600 K, stress is localized at only one location while at 100 K, apart from necking, some secondary crack nucleation and propagation also emerge at some other locations prior to failure (marked by the red rectangles). This might be due to the fact that since the

![Figure 6](https://example.com/fig6.png)

**Fig. 6** The failure mechanism of [100] oriented Si_{0.5}Ge_{0.5} alloy NW at a 100 K and b 600 K for various strain level. Yellow color indicates the distorted cubic zinc blende crystal of Si_{0.5}Ge_{0.5} within the NW, where stress concentration is maximum while violet color indicates the perfect crystal structure of Si_{0.5}Ge_{0.5}
fracture process terminates much earlier at 600 K, the system does not get adequate time to initiate the secondary cracks. Note that the empirical potentials utilized in MD simulations typically cannot properly describe the crack tips during the fracture nucleation process of nanomaterials. Therefore, it may affect the results (identifying the crack tip appropriately). To get more perception of the fracture process of the Si<sub>0.5</sub>Ge<sub>0.5</sub> alloy NW, readers are referred to the movie provided in the supplementary information of this article.

Conclusions

In this investigation, the mechanical properties and failure mechanism of Si<sub>0.5</sub>Ge<sub>0.5</sub> alloy NWs are investigated using molecular dynamics simulation. First, the mechanical properties of Si, Ge, and Si<sub>0.5</sub>Ge<sub>0.5</sub> alloy NWs are predicted and it is found that mechanical properties of Si<sub>0.5</sub>Ge<sub>0.5</sub> alloy NW lie in between Si and Ge NWs. Next, we investigated mechanical characteristics of this alloy by varying different parameters such as temperature, cross-sectional areas, loading directions, and finally, introducing monoatomic vacancy defects by removing Si and Ge atoms randomly from the alloy matrix. Temperature plays a crucial role in regulating the mechanical properties of Si<sub>0.5</sub>Ge<sub>0.5</sub> alloy. The stress-strain curves exhibit typical brittle type failure, and no brittle to ductile transition temperature is detected within the temperature regime considered. Both the ultimate tensile strength and Young’s modulus show a strong inverse relationship with temperature under tensile loading. The reduction of the cross-sectional area contributes to a decline in fracture stress and stiffness of the alloy. The tensile mechanical properties of the alloy exhibit a strong dependency on the crystal orientations in the specified temperature range. One of the key findings of this study is that [111] direction offers the maximum strength while the maximum fracture toughness is obtained in the case of [110] direction, at 300 K. The Young’s modulus is the highest for [110] crystal orientation in the temperature range of 100–200 K, but beyond that, [111] orientation endows the highest elasticity among three crystal directions. Atomic-scale defect, such as the vacancy, also plays a prominent role in dictating mechanical behaviors. Both the failure strength and the elastic modulus demonstrate a strong inverse relationship with increased vacancy concentrations but independent of the type of atoms removed. The failure behaviors corresponding to various strain levels in terms of the shear strain parameter of the alloy are also elucidated for 100 K and 600 K temperatures. Upon stretching, the cross-section eventually resembles the form of a neck like a ductile material. Crack nucleation, propagation, and ultimate failure occur much earlier in 600 K temperatures as compared with 100 K owing to the temperature-induced weakening of the structure. This investigation provides a comprehensive understanding of the tensile mechanical properties and reveals interesting deformation mechanisms of Si<sub>0.5</sub>Ge<sub>0.5</sub> alloy NW and will guide experimental studies and design of high-performance thermoelectric devices.

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Compliance with ethical standards

Conflict of interest  The authors declare that they have no conflict of interest.

References

Amato M, Palummo M, Rurali R, Ossicini S (2014) Silicon–germanium nanowires: chemistry and physics in play, from basic principles to advanced applications. Chem Rev 114:1371–1412
Bin MA, Rao Q, He Y (2014) Effect of crystal orientation on tensile mechanical properties of single-crystal tungsten nanowire. Trans Nonferrous Metals Soc China 24:2904–2910
Callister WD, Rethwisch DG (2018) Materials science and engineering: an introduction. Wiley New York, Hoboken
Cui Y, Lieber CM (2001) Functional nanoscale electronic devices assembled using silicon nanowire building blocks. Science 291:851–853
Cui Y, Wei Q, Park H, Lieber CM (2001) Nanowire nanosensors for highly sensitive and selective detection of biological and chemical species. Science 293:1289–1292
Cui Y, Zhong Z, Wang D, Wang WU, Lieber CM (2003) High performance silicon nanowire field effect transistors. Nano Lett 3:149–152
Dos Santos CL, Piquini P (2010) Diameter dependence of mechanical, electronic, and structural properties of InAs and InP nanowires: a first-principles study. Phys Rev B 81:075408
Eom K, Park HS, Yoon DS, Kwon T (2011) Nanomechanical resonators and their applications in biological/chemical detection: nanomechanics principles. Phys Rep 503:115–163
Fang DQ, Zhang RQ (2011) Size effects on formation energies and electronic structures of oxygen and zinc vacancies in ZnO nanowires: a first-principles study. J Appl Phys 109: 044306–044306

Feng X, He R, Yang P, Rouakes M (2007) Very high frequency silicon nanowire electromechanical resonators. Nano Lett 7: 1953–1959

Georgakakis D, Ziogos OG, Polatoglou HM (2014) Vibrational and mechanical properties of Si/Ge nanowires as resonators: a molecular dynamics study. Phys Status Solidi A 211:267–276

Gordon MJ, Baron T, Dhalluin F, Gentile P, Ferret P (2009) Size effects in mechanical deformation and fracture of cantilevered silicon nanowires. Nano Lett 9:525–529

Haddara YM, Ashburn P, Bagnall DM (2017) Silicon-germanium: properties, growth and applications. In: Springer Handbook of Electronic and Photonic Materials. Springer, Berlin, pp 1–1

Han X et al (2007) Low-temperature in situ large-strain plasticity of silicon nanowires. Adv Mater 19:2112–2118

Hanrath T, Korgel BA (2004) Chemical surface passivation of Ge nanowires. J Am Chem Soc 126:15466–15472

Hochbaum AI, Yang P (2010) Semiconductor nanowires for energy conversion. Chem Rev 110:527–546

Hsin C-L, Mai W, Gu Y, Gao Y, Huang CT, Liu Y, Chen LJ, Wang ZL (2008) Elastic properties and buckling of silicon nanowires. Adv Mater 20:3919–3923

Huang P-H, Fang T-H, Chou C-S (2011) The coupled effects of size, shape, and location of vacancy clusters on the structural deformation and mechanical strength of defective nanowires. Curr Appl Phys 11:878–887

Huheey J, Cottrell T (1958) The strengths of chemical bonds. Butterworths, London

Jing N, Xue Q, Ling C, Shan M, Zhang T, Zhou X, Jiao Z (2012) Effect of defects on Young’s modulus of graphene sheets: a molecular dynamics simulation. RSC Adv 2:9124–9129

Kang K, Cai W (2007) Brittle and ductile fracture of semiconductor nanowires—molecular dynamics simulations. Philos Mag 87:2169–2189

Kang K, Cai W (2010) Size and temperature effects on the fracture mechanisms of silicon nanowires: molecular dynamics simulations. Int J Plast 26:1387–1401

Kim JS, Park SH, Park JH, Lee JS (2006) Molecular dynamics simulation of elastic properties of silicon nanowires. Nanoscale Microscale Thermophys Eng 10:55–65

Kizuka T, Takatani Y, Asaka K, Yoshizaki R (2005) Measurements of the atomistic mechanics of single crystalline silicon wires of nanometer width. Phys Rev B 72:035333

Lajtai EZ (1971) A theoretical and experimental evaluation of the Griffith theory of brittle fracture. Tectonophysics 11:129–156

Lee B, Rudd RE (2007) First-principles calculation of mechanical properties of Si<001> nanowires and comparison to nanomechanical theory. Phys Rev B 75:195328

Lee EK, Yin L, Lee Y, Lee JW, Lee SJ, Lee J, Cha SN, Whang D, Hwang GS, Hipsalgaonkar K, Majumdar A, Yu C, Choi BL, Kim JM, Kim K (2012) Large thermoelectric figure-of-merits from SiGe nanowires by simultaneously measuring electrical and thermal transport properties. Nano Lett 12:2918–2923

Levinshtein ME, Rumyantsev SL, Shur MS (2001) Properties of advanced semiconductor materials: GaN, AlInN, InN, BN, SiC, SiGe. John Wiley & Sons, Hoboken

Li H, Zhang R (2012) Vacancy-defect–induced diminution of thermal conductivity in silicon. EPL Europhys Lett 99: 36001

Liang H, Upmanyu M, Huang H (2005) Size-dependent elasticity of nanowires: nonlinear effects. Phys Rev B 71:241403

Lu W, Lieber CM (2006) Semiconductor nanowires. J Phys D Appl Phys 39:R387–R406

Lu H, Zhang J, Fan J (2011) Molecular dynamics study of the tensile mechanical behavior of metallic nanowires with different orientation [J]. Chin J Solid Mech 32:433–439

Ma J et al (2013) Effects of surface chemical structure on the mechanical properties of Si1–xGe x nanowires. Nano Lett 13:1118–1125

Mingo N, Yang L, Li D, Majumdar A (2003) Predicting the thermal conductivity of Si and Ge nanowires. Nano Lett 3: 1713–1716

Morales AM, Lieber CM (1998) A laser ablation method for the synthesis of crystalline semiconductor nanowires. Science 279:208–211

 Munshi MAM, Majumder S, Motalab M, Saha S (2019) Insights into the mechanical properties and fracture mechanism of cadmium telluride nanowire. Mater Res Express 6:105083

Paulus B, Fulde P, Stoll H (1995) Electron correlations for ground-state properties of group-IV semiconductors. Phys Rev B 51: 10572–10578

Pearson GL, Read WT Jr, Feldmann WL (1957) Deformation and fracture of small silicon crystals. Acta Metall 5:181–191

Pial TH, Rakib T, Mojumder S, Motalab M, Akanda MS (2018) Atomistic investigations on the mechanical properties and fracture mechanisms of indium phosphide nanowires. Phys Chem Chem Phys 20:8647–8657

Plimpton S. Fast parallel algorithms for short-range molecular dynamics. (1993)

Qteish A, Resta R (1988) Thermodynamic properties of Si-Ge alloys. Phys Rev B 37:6983–6990

Rurali R (2010) Colloquium: structural, electronic, and transport properties of silicon nanowires. Rev Mod Phys 82:427–449

Shi-Feng X, Shang-Da C, Ai-Kah S (2011) The effect of atomic vacancies and grain boundaries on the mechanical properties of Si nanowires. Chin Phys Lett 28:066201

Skye A, Schelling PK (2008) Thermal resistivity of Si–Ge alloys by molecular-dynamics simulation. J Appl Phys 103:113524

Smith DA, Holmberg VC, Korgel BA (2010) Flexible germanium nanowires: ideal strength, room temperature plasticity, and bendable semiconductor fabric. ACS Nano 4:2356–2362

Smith DA, Holmberg VC, Lee DC, Korgel BA (2008) Young’s modulus and size-dependent mechanical quality factor of nanoelectromechanical germanium nanowire resonators. J Phys Chem C 112:10725–10729

Stampfli P, Bemennann K (1990) Theory for the instability of the diamond structure of Si, Ge, and C induced by a dense electron-hole plasma. Phys Rev B 42:7163–7173

Stekolnikov AA, Furtmüller J, Bechstedt F (2002) Absolute surface energies of group-IV semiconductors: dependence on orientation and reconstruction. Phys Rev B 65:115318
Stukowski A (2009) Visualization and analysis of atomistic simulation data with OVITO—the open visualization tool. Model Simul Mater Sci Eng 18:015012
Sun X, Fu Z, Xia M, Xu Y (2014) Effects of vacancy defect on the tensile behavior of graphene. Theor Appl Mech Lett 4: 051002
Tang D-M, Ren CL, Wang MS, Wei X, Kawamoto N, Liu C, Bando Y, Mitome M, Fukata N, Golberg D (2012) Mechanical properties of Si nanowires as revealed by in situ transmission electron microscopy and molecular dynamics simulations. Nano Lett 12:1898–1904
Tersoff J (1990) Erratum: modeling solid-state chemistry: interatomic potentials for multicomponent systems. Phys Rev B 41:3248
Tsuzuki H, Rino J, Branicio P (2011) Dynamic behaviour of silicon carbide nanowires under high and extreme strain rates: a molecular dynamics study. J Phys D Appl Phys 44: 055405
Vining CB (1991) A model for the high-temperature transport properties of heavily doped n-type silicon-germanium alloys. J Appl Phys 69:331–341
Vining CB, Laskow W, Hanson JO, Van der Beck RR, Gorsuch PD (1991) Thermoelectric properties of pressure-sintered Sn0. 8Ge0. 2 thermoelectric alloys. J Appl Phys 69:4333–4340
Wang ZG, Li JB, Gao F, Weber WJ (2010) Tensile and compressive mechanical behavior of twinned silicon carbide nanowires. Acta Mater 58:1963–1971
Wang KL, Thomas SG, Tanner MO (1995) SiGe band engineering for MOS, CMOS and quantum effect devices. J Mater Sci Mater Electron 6:311–324
Wang WD, Yi C, Fan K (2013) Molecular dynamics study on temperature and strain rate dependences of mechanical tensile properties of ultrathin nickel nanowires. Trans Nonferrous Metals Soc China 23:3353–3361
Wang Z, Zu X, Gao F, Weber WJ (2008) Atomistic simulations of the mechanical properties of silicon carbide nanowires. Phys Rev B 77:224113
Weakliem PC, Carter EA (1992) Surface and bulk equilibrium structures of silicon-germanium alloys from Monte Carlo simulations. Phys Rev B 45:13458–13464
Wu X, Kulkarni JS, Collins G, Petkov N, Almécia D, Boland JJ, Erts D, Holmes JD (2008) Synthesis and electrical and mechanical properties of silicon and germanium nanowires. Chem Mater 20:5954–5967
Zhang C, De Sarkar A, Zhang R-Q (2011) Inducing novel electronic properties in< 112> Ge nanowires by means of variations in their size, shape and strain: a first-principles computational study. J Phys Condens Matter 24:015301
Zhang J-M, Ma F, Xu K-W, Xin X-T (2003) Anisotropy analysis of the surface energy of diamond cubic crystals. Surf Interface Anal Int J Devoted Dev Appl Tech Anal Surf Interfaces Thin Films 35:805–809
Zhu Y, Xu F, Qin Q, Fung WY, Lu W (2009) Mechanical properties of vapor- liquid- solid synthesized silicon nanowires. Nano Lett 9:3934–3939

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