

Molecular Dynamics Simulation of Fracture Behavior of Two-Dimensional Silicon Germanium Structures: The Effect of Geometrical Defects and Crack Growth

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Abstract

In this study, molecular dynamics simulations were performed using the LAMMPS software to obtain a more precise understanding of the mechanical behavior of silicon–germanium (SiGe) nanostructures. Accordingly, the mechanical properties of SiGe nanosheets were investigated over the temperature range of 100–900 K and in the presence of elliptical defects and their associated branched cracks. The results showed that these nanosheets exhibit higher strength in the armchair direction compared to the zigzag direction, and that increasing temperature leads to a continuous reduction in mechanical properties. It was also found that extension of the branched crack originating from the elliptical defect has a significant effect on reducing fracture toughness. Finally, the mechanical properties were optimized using the particle swarm optimization algorithm. These theoretical findings provide valuable insight into the influence of geometrical defects on the mechanical behavior of SiGe nanosheets and can be useful for defect engineering in two - dimensional materials.

Keywords: Molecular dynamics, Mechanical properties, Fracture toughness, Silicon germanium, Optimization.

1. Introduction

The thermal, mechanical, and electrical properties of carbon-based two-dimensional materials have made them an indispensable part of modern science and technology, attracting extensive attention from researchers in theoretical, simulation, and experimental fields. Since carbon is known as one of the strongest elemental materials, graphene is widely regarded as a suitable representative for a broad range of applications, including nanoelectromechanical systems and nanocomposites [1]. However, because this structure has a zero-band gap and therefore cannot be used as a supercapacitor or transistor in electronic circuits, structural modification through the substitution of other atoms with larger band gaps is employed to enhance its various properties [2].

Given the proximity of carbon to silicon and germanium in the periodic table—and the resulting similarity in their valence electrons—these two elements can serve as suitable substitutes for carbon within the graphene lattice. Semiconductor silicon germanium (SiGe) nanostructures have been employed in recent theoretical studies, and previous research has also examined the properties of SiGe nanotubes [3]. However, considering the distinct characteristics of SiGe nanosheets, further

investigation of this 2D structure is still required. It should be noted that nanosheets, like other materials, are not found as perfect, defect-free single crystals. Therefore, by accounting for structural defects in nanostructures, an appropriate pathway can be established for utilizing these materials on a larger scale and achieving industrial objectives.

In this study, the mechanical properties of SiGe nanosheets are compared using molecular dynamics simulations, with a focus on geometric defects and their dependence on temperature. The mechanical response of SiGe nanostructures containing various geometric defects, as well as the influence of branched cracks originating from these defects, is examined. Accordingly, the mechanical behavior of SiGe nanosheets with two different lattice configurations is evaluated along both the armchair and zigzag directions. In the next stage, the effect of cracks branching from elliptical is investigated. Finally, the fracture toughness of the nanostructures is analyzed, and in the concluding section, the mechanical properties are optimized using the particle swarm optimization algorithm.

2. Molecular dynamics modeling

Molecular dynamics simulations were performed in

this study using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). The interactions between silicon and germanium atoms were described using the Tersoff potential. The hexagonal honeycomb structure of silicon–germanium is illustrated in Figure 1. The two loading directions, armchair and zigzag, correspond to the X and Y axes, respectively. A structure size of $100 \times 100 \text{ \AA}^2$ containing 1472 atoms was considered, enabling the evaluation of the mechanical properties—including Young’s modulus, fracture stress, fracture toughness, and fracture energy—under various conditions. All simulations were conducted under equilibrium conditions. In each case, the system was first equilibrated at constant temperature and pressure using the Nose–Hoover algorithm with a time step of 0.001 ps for a duration of 50 ps. The model was then subjected to uniaxial tensile loading at a strain rate of 0.1 ps^{-1} , while periodic boundary conditions were applied in the in-plane directions. Finally, stress–strain curves were obtained from the simulation data to analyze the mechanical behavior of the structures.

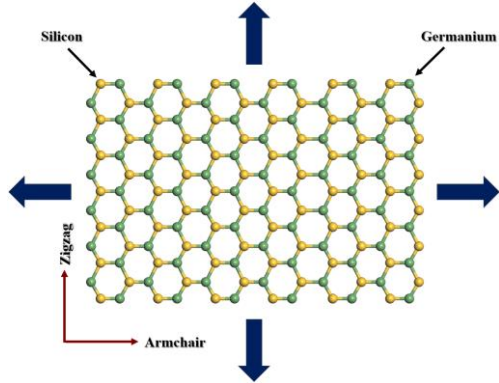


Figure 1. Schematic of the 2D SiGe structure, in which silicon and germanium atoms are arranged as neighboring elements.

3. Results and discussion

To examine the influence of temperature variations from 100 to 900 K, the fracture behavior of SiGe nanosheets was investigated along both the armchair and zigzag directions. As illustrated in Figure 2, increasing the temperature from 100 to 900 K acts as a significant factor affecting the nanostructures. Moreover, SiGe nanosheets exhibit higher resistance under tensile loading in the armchair direction compared to the zigzag direction. The peak stress represents the onset of unstable crack propagation and the complete rupture of the atomic network. Since increasing temperature leads to an expansion of the Si–Ge bond length, the corresponding reduction in bond energy weakens the atomic connections, thereby reducing the mechanical resistance of the two-dimensional structure [4].

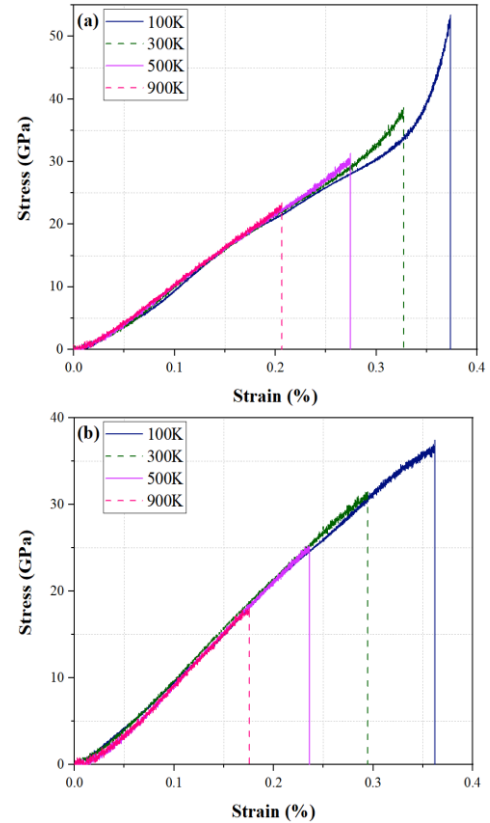


Figure 2. Stress-strain variations of SiGe structures: a) Armchair direction, b) Zigzag direction.

According to the results shown in Figure 3, both Young’s modulus and fracture stress decrease as the temperature increases from 100 to 900 K. Furthermore, the mechanical properties in the armchair direction were consistently higher than those obtained under zigzag loading. As temperature increases, the atomic spacing expands, which reduces the interatomic interaction energy and consequently leads to a decline in mechanical properties. Variables such as temperature, which alter the distance and forces between atoms, can significantly influence the mechanical response. Therefore, increasing temperature weakens atomic bonding and chemical interactions, resulting in reduced mechanical strength.

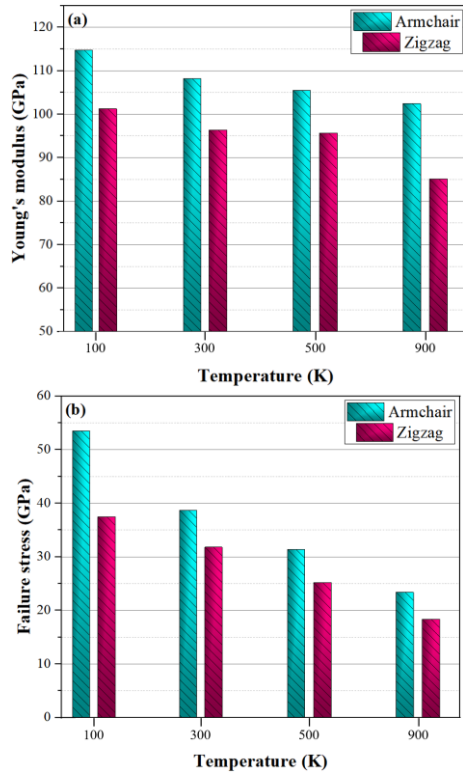


Figure 3. Mechanical properties of SiGe nanostructures for two configurations: a) Young's modulus, b) Fracture stress.

Figure 4 presents the obtained fracture toughness values. The direct relationship between fracture toughness and crack length indicates that fracture toughness increases as the crack becomes longer. Physically, larger cracks possess greater surface area exposed to stress, making them more susceptible to further propagation. Increasing crack length intensifies the stress concentration at the crack tip, facilitating crack growth within the material [5].

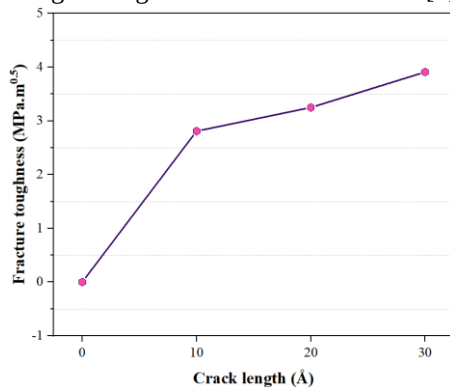


Figure 4. Variations in fracture toughness for structures containing an elliptical defect and a branched crack.

The crack length and geometric defect area were used as input variables for evaluating and optimizing the mechanical properties of SiGe nanosheets. Specifically, these inputs were used to determine the optimal values of Young's modulus, enabling a more precise characterization of the material's response to

structural defects. Figure 5 presents the three-dimensional plot of Young's modulus variations as a function of defect area and branched crack length. The optimal value obtained for Young's modulus corresponds to a defect area of 20.5 Å² and a crack length of 6.52 Å, yielding a modulus of 75.18 GPa. It is important to note that, since defects inherently reduce mechanical performance, the reported optimal values represent the defect geometries that cause the least degradation, rather than properties exceeding those of the pristine structure.

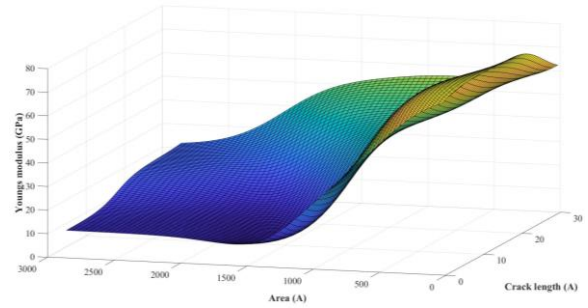


Figure 5. Three-dimensional plots of Young's modulus as functions of geometric defect area and crack length.

4. Conclusion

In the present study, the mechanical properties and fracture behavior of SiGe nanosheets were examined as functions of temperature and geometric defects. Using molecular dynamics simulations, branched cracks originating from elliptical holes were modeled. The results showed that the mechanical properties of SiGe structures decrease with increasing temperature. Also, the analysis of branched cracks revealed that increasing crack length acts as an effective parameter in determining fracture behavior. Finally, to identify the optimal mechanical performance of SiGe nanosheets, the particle swarm optimization algorithm was employed using crack length and defect area as input parameters.

5. References

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