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Mechanical Response of Buckled Germanene: Influence of Temperature, Strain Rate and Point Defects

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ABSTRACT

Germanene, a two-dimensional material with a unique buckled honeycomb structure, has recently drawn attention for its potential in nanoelectromechanical systems (NEMS) and advanced nano-devices. In this work, we explore how temperature, strain rate, and point defects influence its mechanical performance through molecular dynamics simulations. The findings show that as temperature rises, the fracture stress, strain, and elastic modulus drop sharply by as much as 66% due to stronger atomic vibrations and thermal softening. In contrast, faster strain rates significantly improve these properties, enhancing strength by nearly 45% because atoms have less time to relax. The presence of point vacancies, even in small amounts, weakens the structure considerably, as these defects act as stress concentrators that trigger early fracture. Interestingly, a clear anisotropy is observed: the zigzag direction offers higher strength, while the armchair direction remains more flexible. Overall, the study provides valuable insights into how germanene responds under different conditions and highlights its promise as a durable and tunable material for next-generation nanoelectronic and electromechanical devices.

Keywords: Germanene, Mechanical properties, NEMS, Anisotropy.

1. Introduction

As nanotechnology continues to advance, there is a growing demand for nanoelectromechanical systems (NEMS) like nanoresonators, nanocomposites, and devices for energy harvesting and conversion at the nanoscale. These are being developed to address the drawbacks of traditional microscale systems. Yet, a major obstacle is the tendency of current NEMS to suffer from mechanical failure [1]. To overcome this, researchers are exploring nanoscale materials with extremely high fracture stress and excellent electronic performance. Among the options, two-dimensional (2D) materials stand out because of their unique electronic features, high surface-to-volume ratio, and remarkable mechanical durability [2]. Inspired by the groundbreaking exfoliation of graphene and its remarkable capabilities, researchers soon recognized its limitations: the absence of a bandgap, which restricts its effectiveness in transistors and logic circuits [3]. These drawbacks have encouraged the search for other 2D materials like silicene, h-BN, GaN, MoS_2, and ZnO [4].

Among emerging two-dimensional materials, germanene a group-IV honeycomb analogue has attracted considerable interest owing to its compatibility with existing semiconductor technology and its remarkable electronic, magnetic, and thermoelectric properties[5]. Unlike graphene, germanene has a buckled structure with mixed sp^2/sp^3 hybridization, giving it a chemically active surface and tunable electronic properties. Its bandgap can be adjusted through chemical functionalization or external electric fields, making it promising for field-effect transistors and optoelectronics [6]. Moreover, germanene nanoribbons further enhance its versatility, where edge doping or functionalization can switch their behavior between semiconducting, metallic, or half-metallic states, while also influencing magnetic ordering. Such flexibility is valuable for multifunctional NEMS applications [7]. Therefore, studying the mechanical properties of germanene nanosheet is essential to understand its potential for use in next-generation devices and technologies.

The mechanical properties of 2D materials are highly sensitive to temperature, strain rate, and [4], [8], [9]. Rising temperature weakens their strength as atomic vibrations disturb the lattice, leading to thermal softening, though the extent varies with structural features like ripples or anharmonicity. Strain rate generally enhances fracture stress and fracture strain by limiting atomic relaxation. On the other hand, point vacancies reduce performance by lowering the elastic modulus, fracture strength, and failure strain, with

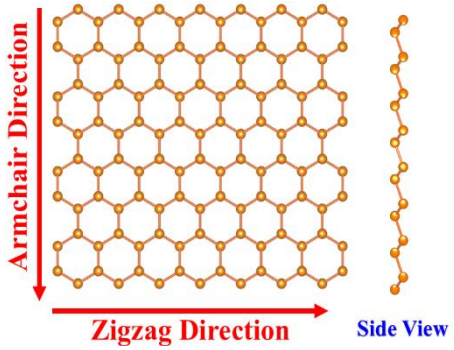

Fig.1: Buckled honeycomb structure of germanene showing zigzag and armchair directions.

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higher concentrations further intensifying this effect as observed in Ti_2C MXene [10]. While germanene shows strong potential for nano- and optoelectronic devices, its mechanical response to temperature, defects, and strain rate still remains underexplored, requiring detailed investigation for reliable applications.

Classical molecular dynamics (MD) simulations have become a reliable way to study nanomaterials, producing results nearly consistent with experiments. In this work, we use MD to explore how temperature, strain rate, and point vacancies affect germanene's mechanical behavior, modeled with the Tersoff potential. The stress–strain response shows an initial linear region, then nonlinear, and finally a steeper linear rise before brittle fracture. Fracture stress decreases with rising temperature due to enhanced atomic vibrations, while at 300 K pristine germanene shows higher strength at faster strain rates from limited atomic relaxation. Point vacancies, however, reduce strength by acting as stress concentrators. Strong anisotropy is observed: zigzag offers higher strength, whereas armchair provides better stretchability.

2. Computational Method

Molecular dynamics simulations were performed using the LAMMPS package to study the tensile mechanical properties of monolayer germanene. The system was modeled as a buckled honeycomb lattice of Ge atoms, constructed in a simulation box of approximately 10 nm × 10 nm in the in-plane directions. To avoid artificial interactions in the out-of-plane direction, a vacuum region of about 20 Å was introduced along the *z*-axis. For the calculation of stress, an effective thickness of 4.22 Å was assumed for the germanene sheet. The interactions between Ge atoms were described by the Tersoff potential [11]. This potential form includes both two-body and three-body terms and is well suited for describing covalent bonding and bond breaking processes in germanene. The simulation time step was set to 1 fs throughout all runs.

Prior to mechanical loading, the structure was relaxed using the conjugate gradient (CG) method to remove residual stresses. After minimization, equilibration was performed in three steps. First, a short run under the microcanonical ensemble (NVE) was used to stabilize atomic velocities. Second, the system was equilibrated in the isothermal–isobaric ensemble (NPT) at 300 K and 1 bar to release any in-plane stresses. Finally, the canonical ensemble (NVT) was employed to thermalize the system at the desired target temperature.

Uniaxial tensile loading was then applied by uniformly deforming the simulation box using the fix deform command in LAMMPS. Both armchair and zigzag Directions of the lattice were tested by aligning the loading axis along the x or y direction of the simulation box. During deformation, the system temperature was maintained by the Nosé–Hoover thermostat in the NVT ensemble. Uniaxial tensile strain was applied to monolayer germanene using LAMMPS, allowing the calculation of elastic modulus, fracture stress, and fracture strain. Simulations were performed at temperatures from 100 K to 600 K and strain rates between 0.0001 ps^{-1} and 0.0125 ps^{-1}, enabling a detailed analysis of how temperature and loading rate influence its mechanical behavior. The structural stability under different conditions was analyzed and the influence of atomic vacancies was also explored, with vacancy concentrations ranging from 0.2% to 1% to assess their impact on the tensile-mechanical behavior of germanene. The tensile stress–strain behavior was extracted from the virial stress tensor. The stress was averaged over the entire system volume and converted into GPa using the effective thickness of 4.22 Å. From these stress–strain curves, the elastic modulus, fracture strength, and fracture strain were determined.

3. RESULT AND DISCUSSIONS

2D materials such as germanene, silicene, SiGe, h-BN, and MoS_2 are emerging as promising nanomaterials for advanced applications in environments that may vary drastically [4]. A key challenge is their stability at extreme temperatures, which is critical for NEMS, solar cells, nanosensors, aerospace systems, fuel cells, and energy-harvesting devices that require durable structures. To address this, we investigate the uniaxial tensile mechanical properties of monolayer germanene depending on temperature from 100K to 600K at fixed strain rate 0.001 ps^{-1}, with the stress–strain behavior presented in Fig. 2(a) and 2(b).

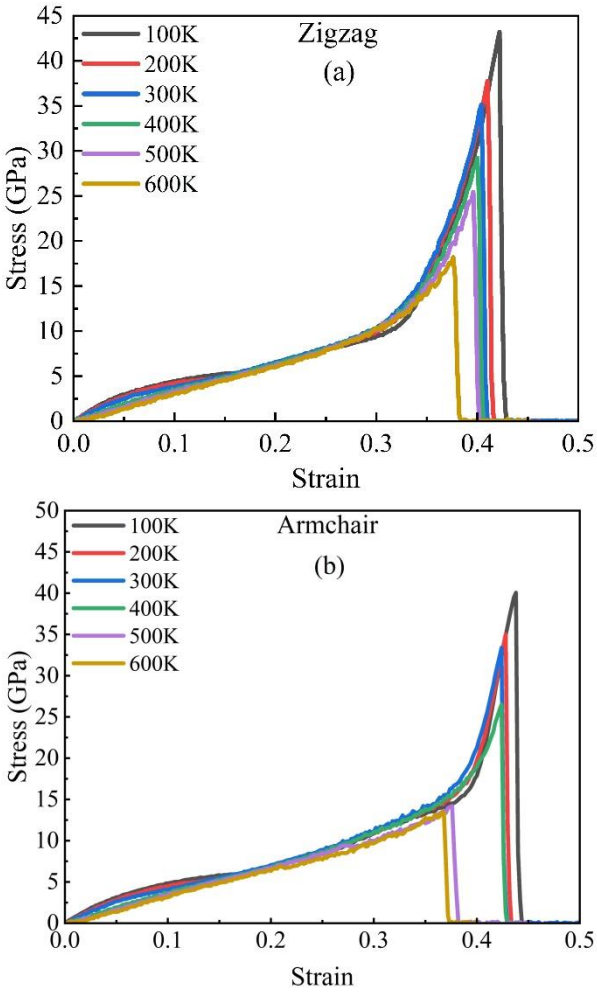

Fig.2: Stress–strain response of germanene as a function of temperature along the (a) zigzag and (b) armchair directions.

The response is initially linear due to elastic bond stretching, becomes nonlinear as bonds distort, and regains a near-linear character before brittle fracture. With increasing temperature, atomic vibrations intensify, weakening

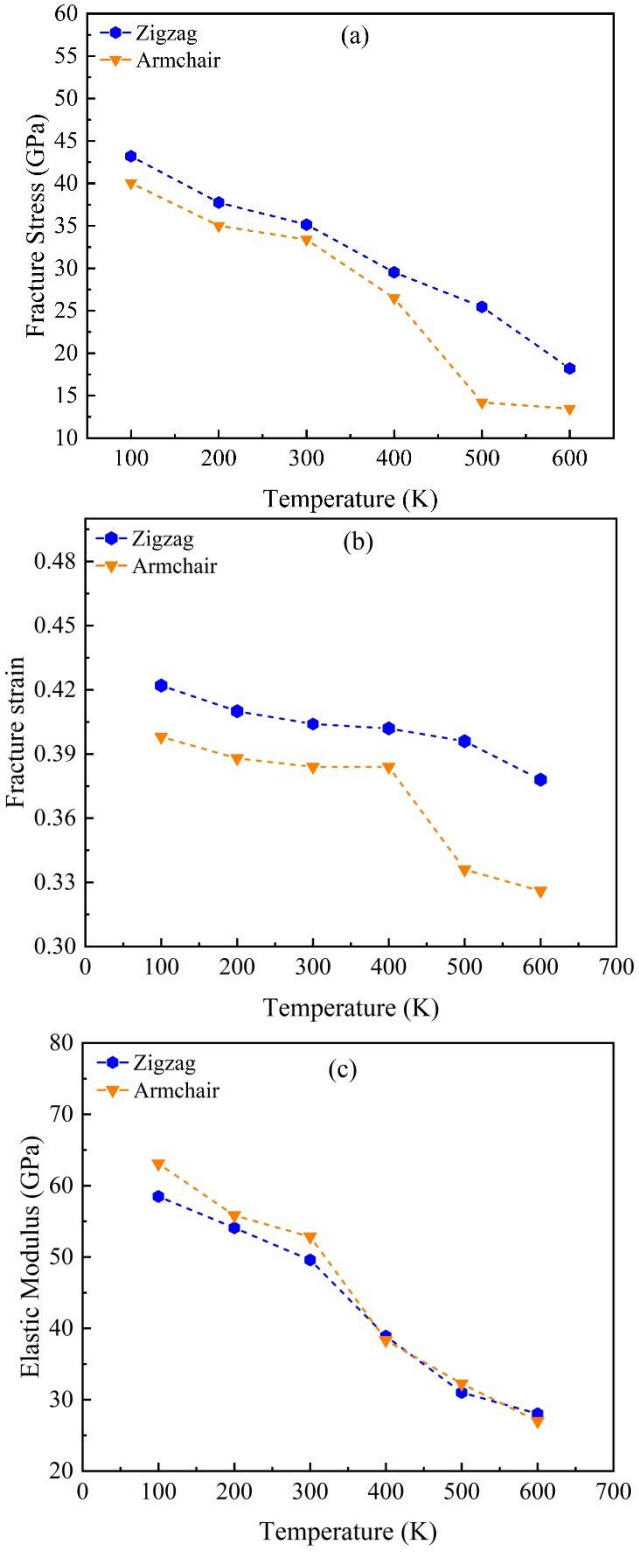

Fig.3: Variation of mechanical properties of germanene under different temperature: (a) fracture stress, (b) fracture strain, and (c) elastic modulus.

interatomic bonds and lowering the energy barrier for rupture. Consequently, strain-hardening observed at low temperatures diminishes and vanishes above 500 K, where thermal agitation dominates bond stiffness and leads to earlier failure.

Fig. 3(a-c) shows the mechanical attributes as a function of temperature. In Fig. 3(a) that the fracture stress of germanene decreases steadily with temperature, from 43.2 GPa to 18.2 GPa in the zigzag direction and 40.1 to 13.5 GPa in the armchair direction with corresponding reductions of 57.9% and 66.3% varying temperature from 100K to 600K respectively. Fig. 3(b) shows that the fracture strain of germanene decreases with temperature, from 0.422 to 0.378 in the zigzag direction and 0.438 to 0.366 in the armchair direction, corresponding to reductions of 10.4% and 16.4% as the temperature increases from 100 K to 600 K. Fig. 3(c) shows that the elastic modulus of germanene decreases with temperature, dropping from 58.5 GPa to 49.6 GPa and 28.0 GPa in the zigzag direction, and from 63.1 GPa to 52.8 GPa and 27.0 GPa in the armchair direction as the temperature increases from 100 K to 300 K and 600 K, respectively. These reductions of more than 50% and the convergence beyond 400 K indicate that thermal vibrations progressively suppress orientation-dependent stiffness. Overall, increasing temperature leads to systematic reductions in fracture stress, fracture strain, and elastic modulus, highlighting the progressive weakening of germanene's mechanical properties under thermal effects.

To further understand the mechanical response of germanene, the effect of strain rate was investigated at 300 K. Strain rate variation is important because it reveals the time-dependent deformation behaviour of 2D materials, indicating whether their mechanical response is rate sensitive. The stress–strain curves in Fig. 4(a) and 4(b) show that the initial elastic portions largely overlap for all strain rates, confirming that the elastic modulus remains nearly independent of loading rate in both zigzag and armchair

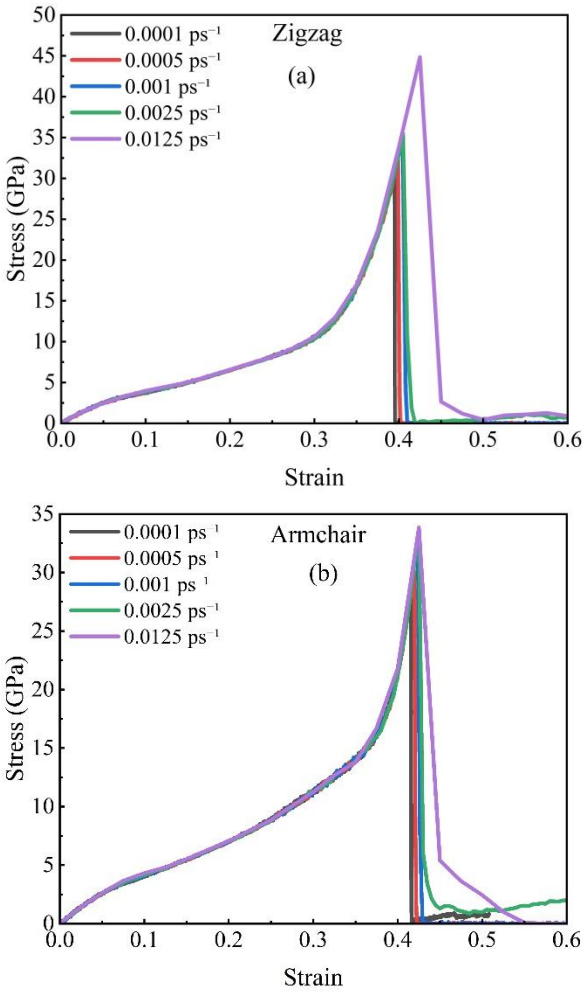

Fig.4: Stress–strain response of germanene as a function of strain rate of along the (a) zigzag and (b) armchair directions.

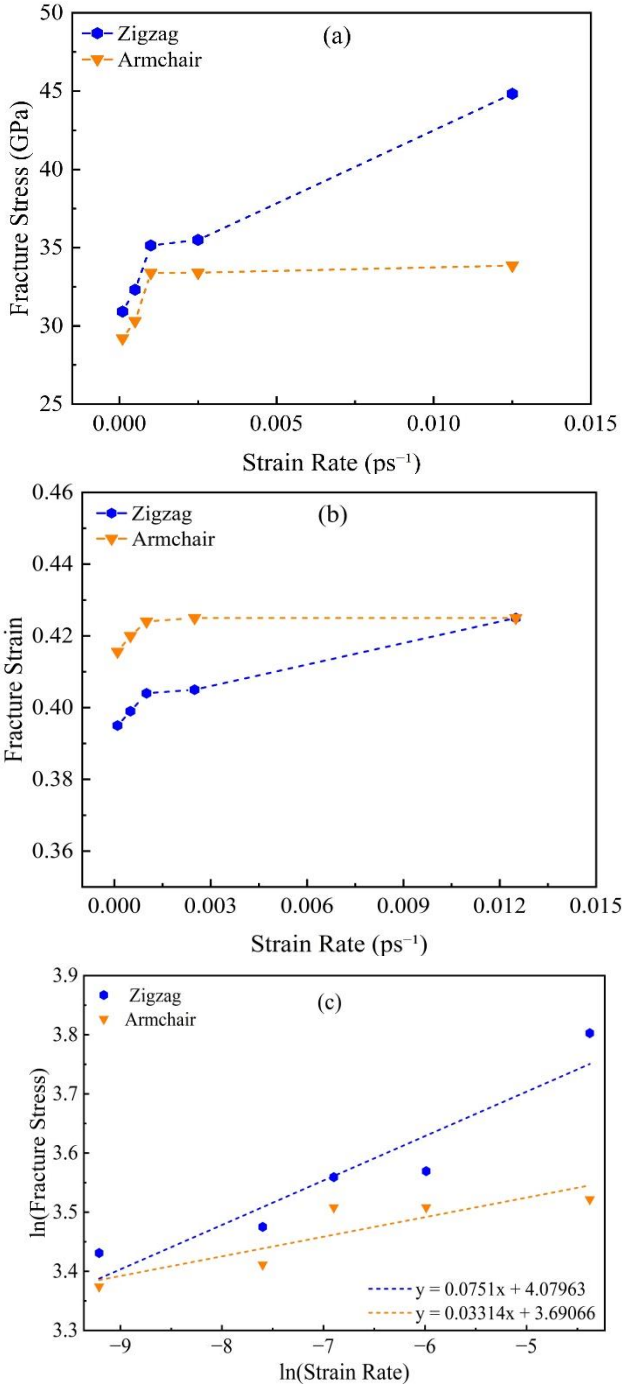

Fig.5: Mechanical properties of germanene depending on strain rate variation (a) fracture stress, (b) fracture strain, and (c) elastic modulus.

orientations. However, clear differences emerge at higher strains. With increasing strain rate, both fracture stress and fracture strain improve, while the brittle failure mode persists. This strengthening can be attributed to limited atomic relaxation at high loading rates. At slower strain rates, atoms have sufficient time to rearrange and relieve local stress concentrations, leading to earlier bond rupture and lower strength. In contrast, under rapid loading, the reduced time for atomic motion prevents relaxation, allowing more bonds to be loaded simultaneously, which delays failure and enhances both strength and ductility.

The effects are summarized in Fig. 5(a-c). Fig. 5(a) shows that the fracture stress increases with strain rate, rising from 30.9 GPa to 44.8 GPa in the zigzag direction and from 29.2

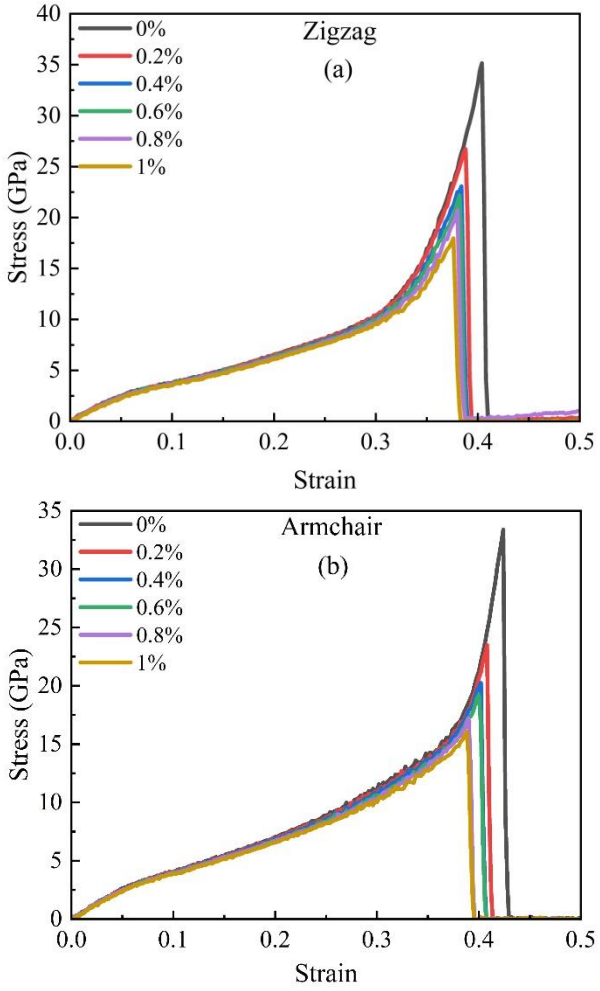

Fig.6: Stress–strain response of germanene with varying defect concentration along the (a) zigzag and (b) armchair directions.

GPa to 33.8 GPa in the armchair direction as the strain rate increases from 0.0001 ps⁻¹ to 0.0125 ps⁻¹, corresponding to gains of 44.9% and 15.8%, respectively.

Fig. 5(b) shows that the fracture strain increases with strain rate, rising from 0.395 to 0.425 in the zigzag direction and from 0.416 to 0.425 in the armchair direction as the rate increases from 0.0001 ps⁻¹ to 0.0125 ps⁻¹, corresponding to increments of 7.6% and 2.2%, respectively. These results indicate stronger rate sensitivity along the zigzag orientation. he strain rate sensitivity of germanene was further analyzed to quantify the relationship between fracture stress and applied strain rate. Using the Arrhenius-type relation:

$$\dot{\varepsilon} = A\sigma^{\frac{1}{m}} exp\left(\frac{-Q}{RT}\right) \quad (1)$$

By applying the natural logarithm to both sides of Equation 2 and considering the temperature to remain constant throughout the deformation. The expression can be simplified as follows:

$$ln(\dot{\varepsilon}) = ln(A) + \frac{1}{m} ln(\sigma) - \frac{Q}{RT} \quad (2)$$

$$m = \frac{\partial ln(\dot{\varepsilon})}{\partial ln(\sigma)} \quad (3)$$

Fig. 5(c) shows the logarithmic variation of fracture stress with strain rate. The fitted slopes give strain-rate sensitivities of 0.033 in the armchair and 0.075 in the zigzag direction, indicating that zigzag is about twice as responsive due to its anisotropic bonding arrangement.

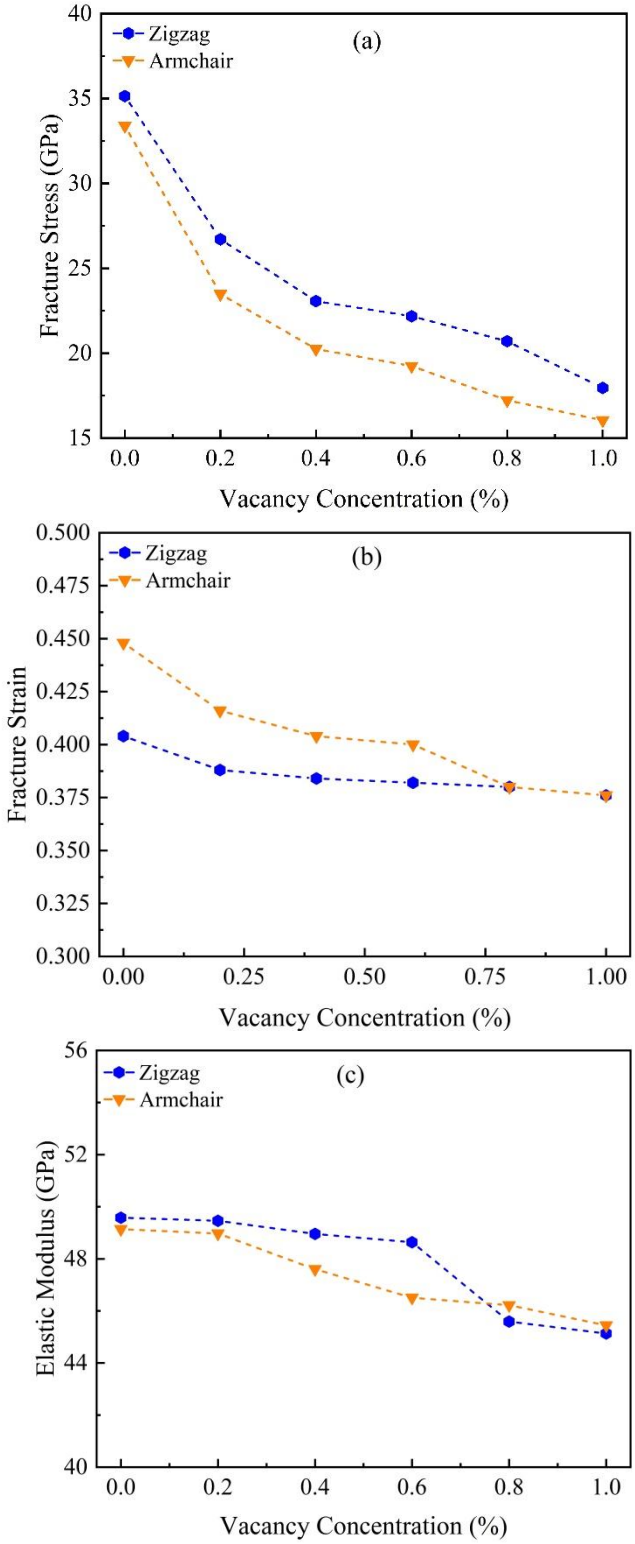

Fig.7: Mechanical properties of germanene under different vacancy concentrations: (a) fracture Stress (b) fracture Strain and (c) elastic Modulus of germanene.

The fabrication of pristine germanene is nearly impossible, and various structural defects introduced during synthesis can significantly affect its mechanical performance. Among these, vacancies are particularly important as they act as stress concentrators, reducing the material's ability to sustain load. In molecular dynamics simulations, vacancy defects can be introduced in controlled concentrations, and their effect on mechanical properties can be systematically analyzed. Fig. 6(a) and 6(b) show the stress–strain curves of germanene with increasing random vacancy concentration 0.2% to 1.0% with fixed strain rate 0.001 ps^{-1} at 300 K. The initial elastic portion remains almost unchanged, confirming that small defects do not strongly affect stiffness. However, both fracture stress and fracture strain decrease steadily with more vacancies, since missing atoms introduce stress concentrations that weaken bonds and trigger earlier failure.

Figure 7(a–c) illustrates the effect of point vacancies on the mechanical properties. Fig. 7(a) illustrates the effect of defect percentage on fracture stress of 2D germanene. Pristine germanene reaches 35.14 GPa in the zigzag direction and 33.39 GPa in the armchair direction. With vacancy concentration rising to 1%, the strength falls nearly by half, with zigzag always slightly stronger than armchair. Fig. 7(b) shows that fracture strain follows the same trend, dropping from 0.404 and 0.424 in the pristine sheet to 0.376 and 0.388 at 1% vacancies. The armchair direction remains a little more stretchable, though this advantage decreases as defects accumulate. Fig. 7(c) presents the elasti modulus, which declines moremoderately from 49.58 GPa and 48.57 GPa in the pristine sheet to about 45 GPa in both directions at 1% vacancy concentration, indicating progressive lattice softening.

These results reveal that vacancies strongly reduce fracture stress and ductility while also weakening stiffness, with zigzag showing slightly higher strength and armchair retaining slightly higher ductility at low defect levels. At higher vacancy concentrations, these orientation-dependent differences diminish due to the homogenizing effect of random defects.

4. Conclusion

This study highlights the critical role of external factors and structural imperfections in shaping the mechanical performance of buckled germanene. The contrasting responses to temperature, strain rate, and vacancy defects underscore its tunability, offering valuable guidance for defect engineering and device design. The observed anisotropy between armchair and zigzag orientations further suggests direction-dependent applications, where strength or elasticity can be selectively utilized. These findings not only advance the fundamental understanding of germanene mechanics but also strengthen its candidacy for integration into nanoelectromechanical and nanoelectronic systems. Looking ahead, tailoring germanene's mechanical response could open pathways for durable, high-performance components in next-generation nanoscale technologies.

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6. NOMENCLATURE

Symbol	*Meaning*	*Unit*
T	Temperature	(K)
P	Pressure	(Pa)
$\dot{\varepsilon}$	strain rate	(Ps^{-1})
σ	Stress	(GPa)
A	Arrhenius Constant	($ps^{-1}\cdot GPa^{-n}$)
Q	Activation Energy	(J/mol)
R	Universal Gas Constant	(J/(ml.K))
m	Strain rate sensitivity	Dimension less