

DEPENDENCE OF THE TENSILE BEHAVIOR OF SINGLE GRAPHENE SHEET ON TEMPERATURE AND STRAIN RATE

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Introduction

Graphene sheets—one-atom-thick two-dimensional (2D) layers of sp²-bonded carbon— have received great interest since their discovery by Novoselov et al. [1] because of their unusual electronic properties, extraordinary electronic transport properties, high thermal conductivity properties and exceptional mechanical properties [2-4]. However, to date, investigations into the effects of temperature and strain rate on the mechanical properties of graphene are still lacking because of experimental difficulties. Numerical methods, such as empirical molecular dynamics (MD) simulation can be used to derive both equilibrium and nonequilibrium properties of materials under extreme environmental settings quantitatively or qualitatively.

Simulation Method

In our work, dependences of the tensile behavior of single graphene sheets on temperature and strain rate were investigated by means of MD simulations with Tersoff-Brenner bond-order interatomic potential, which is specially suited for carbon-based systems, such as diamond, graphite, fullerenes, nanotubes and graphene, and has been used in a wide variety of scenarios with results in agreement with experimental observations. Both armchair and zigzag graphene sheets were considered to compare their difference. The models used in the simulation are shown in Fig.1.

Firstly, temperature (0K-3000K) dependences of tensile mechanical properties for armchair and zigzag single graphene sheets at a strain rate of 1×10^9 1/s were studied. The difference of the tensile

mechanical properties between the armchair and zigzag sheets at different temperature was also studied and analyzed. Secondly, molecular dynamics simulations of strain rate (1×10^8 1/s~ 5×10^{11} 1/s) effects on the tensile mechanical properties were performed at 0K.

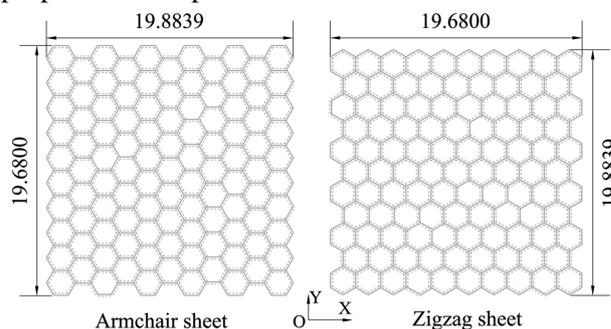


Fig.1 Graphene models used in the simulation

Results and Discussion

Fig.2 and Fig.3 give the results of Young's modulus and tensile strength of the armchair and zigzag graphene sheets as a function of temperature.

The simulation results indicate that the tensile mechanical properties of the sheets are strongly dependent on the temperature. The Young's modulus, tensile strength and fracture strain of the two chiral sheets all decrease significantly with increasing temperature, as shown in Fig.2 and Fig.3. It is also found that the mechanical anisotropy of the sheets is affected by the temperature. When the temperature is lower than 600K, the mechanical properties of armchair sheets are superior to that of zigzag ones. However, when the temperature is higher than 600K, this superiority diminishes gradually and even turns into inferiority, especially at high temperature.

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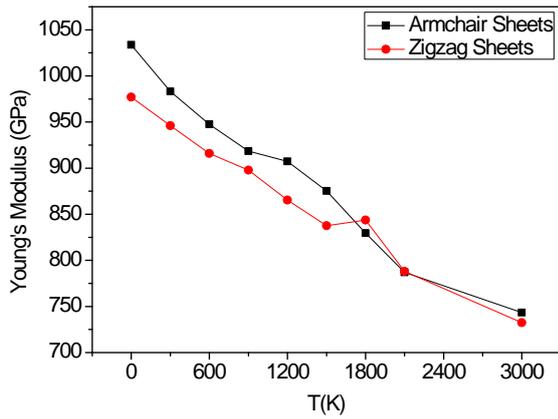


Fig.2 Young's modulus of armchair and zigzag single graphene sheets vs. temperature

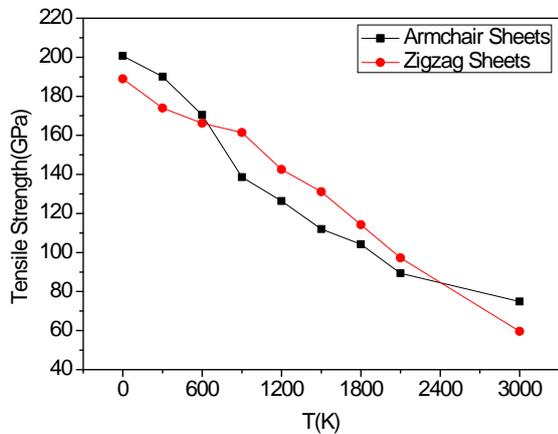


Fig.3 Tensile strength of armchair and zigzag single graphene sheets vs. temperature

Fig.4 and Fig.5 show the effect of strain rate on the Young's modulus and tensile strength of armchair and zigzag graphene sheets at temperature 0K. The results indicate that the tensile mechanical properties of the sheets are also strongly dependent on the strain rate. When the strain rate is lower than 5×10^9 1/s, the Young's moduli of both chiral graphen sheets decrease with strain rate, but the tensile strength is not very sensitive, as shown in Fig.4 and Fig.5. When the strain rate is higher than 5×10^9 1/s, higher strain rates lead to higher Young's modulus, tensile strength and corresponding tensile strain. In addition, the deformation mechanisms of graphene sheets under tension change with the temperature and strain rate.

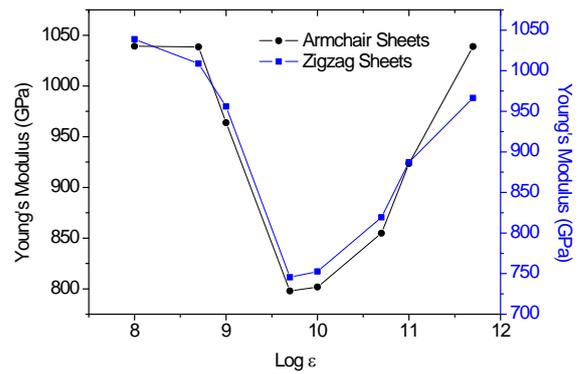


Fig.4 Young's modulus of armchair and zigzag single graphene sheets vs. strain rate

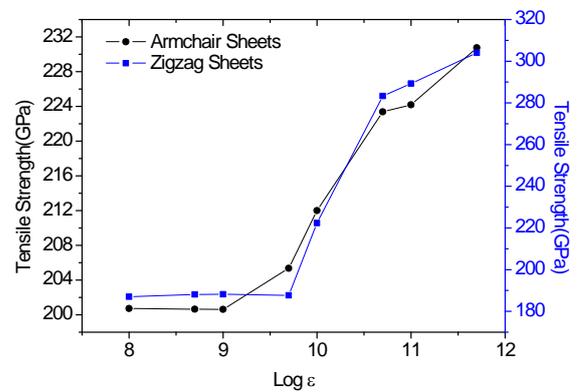


Fig.5 Tensile strength of armchair and zigzag single graphene sheets vs. strain rate

Conclusion

To conclude, the tensile mechanical properties of graphene sheets are strongly dependent on the temperature and strain rate. However, the strain rate effect is relatively small, far less obvious than the temperature effect. These results may provide valuable guiding principles to optimize and develop novel nanoscale devices and new materials concepts.

References

- [1]K. S. Novoselov, A. K. Geim, S. V. Morozov, et al. Electric field effect in atomically thin carbon Films. Science, 2004, 306(22): 666-669.
- [2]Fang Liu, Pingbing Ming, Ju Li. Ab initio calculation of ideal strength and phonon instability of graphene under tension [J]. Physical Review B, 2007, 76: 064120.
- [3] Changgu Lee, Xiaoding Wei, Jeffrey W. Kysar, et al. Measurement of the Elastic Properties and Intrinsic Strength of Monolayer Graphene [J]. Science, 2008, 321(5887): 385-388.
- [4] Sasha Stankovich, Dmitriy A. Dikin, Geoffrey H. B. Dommett, Kevin M. Kohlhaas, Eric J. Zimney, Eric A. Stach, et al. Graphene-based composite materials. Nature, 2006, 422: 282-286.