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Atomic-Scale Analysis of Physical Strength and Phonon Transport Mechanisms of Monolayer *β*-Bismuthene

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Supporting Information

Virial Stress Formulation

The atomic stress in our simulation is calculated using Virial stress theorem which stands as,

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

In this theorem, the summation is performed over all the atoms occupying a volume Ω, $\dot{m}_i$ presents the mass of atom i, $\otimes$ is the cross product, $\dot{u}_i$ is the time derivative, which indicates the displacement of the atom with respect to a reference position, r_{ij} represents the position vector of the atom, and f_{ij} is the interatomic force applied on atom i by atom j .

Table 1. Parameter for Stillinger Weber (SW) potential for beta bismuthene. Note that only epsilon and sigma have unit and other parameters are unitless.

Element 1	Element 2	Element 3	ϵ (eV)	σ (Angstrom)	a	λ	γ	$\cos\Theta_o$	A	B	P	Q	tol
Bi	Bi	Bi	1	0.552	6.690	10.574	1	-0.016	6.805	462.978	4	0	0.0

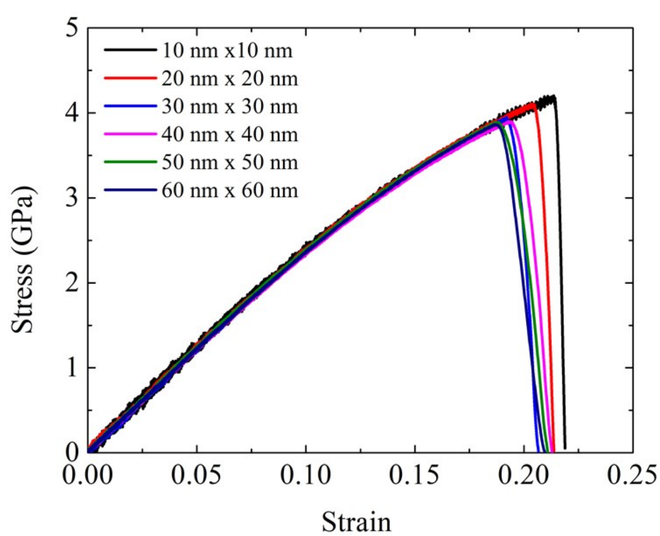

FIGURE S1. Demonstartion of tensile properties of beta bismuthene along with armchair direction considering different system size size at 300K at a strain rate of 10^9 (s^{-1})

To check the convergence of the mechanical properties with system size, we carried our tensile simulation of beta bismuthene at 300K considering 6 different system sizes, such as 10 nm x 10 nm, 20 nm x 20 nm, 30 nm x 30 nm, 40 nm x 40 nm, 50 nm x 50 nm, and 60 nm x 60 nm using a strain rate of 10^9 (s^{-1}). It is quite evident from Fig.S1 that any simulation cell sizes larger than 20 nm x 20 nm has negligible influence on the tensile properties such as UTS, fracture strain and, YM; hence we have reported all the tensile properties considering a system size of 40 nm x 40 nm, which allows to perform the study within a reasonable computational time.