Supplementary Information (SI) for Nanoscale.

Supporting Information

Anisotropy deformation behavior of multi-layer black phosphorus

Zihan Li[1,2], Guangrui Zhao[2], Xiaosong Zhang[2], Yongda Yan[1,2], Yanquan Geng[1,*]

[1] *The State Key Laboratory of Robotics and Systems, Robotics Institute, Harbin Institute of Technology, Harbin, Heilongjiang 150080, P.R. China*

[2] *Center for Precision Engineering, Harbin Institute of Technology, Harbin, Heilongjiang 150001, P.R. China*

** Corresponding author. Tel.: +86-0451-86412924. E-mail: gengyanquan@hit.edu.cn (Y. Q. Geng)*

DFT Calculations

The initial crystal structure model of b-P was constructed using Materials Studio software, providing a basic framework for subsequent theoretical calculations. Subsequently, systematic calculations were performed using the Vienna Ab-initio Simulation Package (VASP) software [1,2]. In the calculation process, the Projected Augmented Wave (PAW) method was used to handle electron-ion interactions. Within the framework of the Generalized Gradient Approximation (GGA), the Perdew-Burke-Ernzerhof (PBE) functional was implemented for first-principles Density Functional Theory (DFT) calculations, so as to accurately describe the electronic structure and energy properties of the system [3–5]. Regarding the setting of calculation parameters: the cutoff energy for the plane-wave basis set was uniformly set to 450 eV to ensure the completeness of the basis set. The structure optimization followed strict convergence criteria: the system was considered to reach the lowest-energy stable structure when the residual force on all atoms was less than 0.01 eV/Å and the energy convergence threshold for the self-consistent iteration of the Kohn-Sham equations reached 10^{-4} eV. For the integration of the Brillouin zone, an 8×1×6 Monkhorst-Pack k-point grid was used for sampling to balance calculation accuracy and efficiency [6]. For the important van der Waals interactions in layered materials, dispersion correction was implemented via the DFT-D3 method proposed by Grimme, ensuring the accurate description of interlayer interactions [7].

The relationship between energy and interlayer spacing during the sliding process is shown in Fig. S1(a). By analyzing the energy-interlayer spacing curves of each sliding step, the minimum energy point $E_{\mathrm{min,X}}$, the minimum energy of the initial state $E_{\mathrm{min,0}}$ and E_{Inf} can be determined respectively. The variation trends of E_s and E_c values corresponding to different sliding step numbers are shown in Fig. S1(b). Both curves exhibit a significant periodic wavelike variation characteristic. Characteristic energy extreme points appear in Step 3 and Step 7: the single-atom sliding energy barrier reaches the maximum value of E_s=0.66eV/atom here; while the cleavage energy achieves the minimum value of E_c=0.87eV/atom at these points.

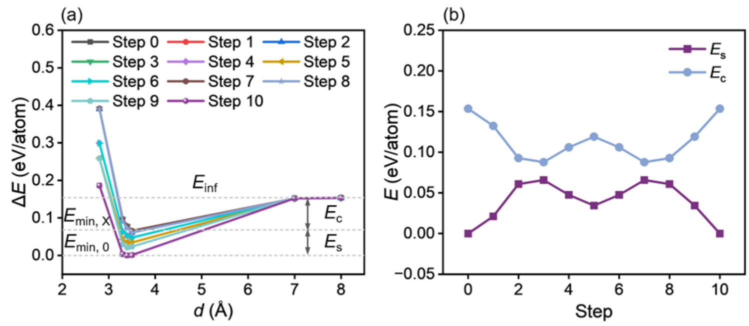

Fig. S1. The variation of E_s and E_c during the slip process

MD simulation

Table S1 Mechanical properties of muti-layered b-P

Orientation	Strain rate (%)	Young's modulus (Gpa)	Fracture strength (Gpa)	Fracture strain (%)
Zigzag	5×10^{8}	105.4	7.7	14.3
Armchair	5×10^{8}	22.3	3.8	23.2

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