Minwoong Joe[1]
Jinhwan Lee[1], and Changgu Lee[1, 2]
[1] School of Mechanical Engineering, Sungkyunkwan University, 2066 Seobu-ro, Jangan-gu, Suwon 440-746, Republic of Korea
[2] SKKU Advanced Institute of Nanotechnology, Sungkyunkwan University, 2066 Seobu-ro, Jangan-gu, Suwon 440-746, Republic of Korea

mjoe122@gmail.com

Dominant in-plane cleavage direction of $CrPS_4$ monolayer

In-plane cleavage directions of 2D crystals are displayed and often well-defined in their flakes exfoliated by the widely-used scotch-tape method. Here, we investigate the correlation between dominant in-plane cleavage direction and elastic properties in different directions. $CrPS_4$ flakes show a preferential in-plane cleavage direction of 67.5°, corresponding to <110> direction. To explain it, we calculated directional dependence of Young's modulus and fracture energy using first-principles density functional theory calculations. We found that fracture energy is directly relevant to the in-plane cleavage direction of $CrPS_4$. Our study can provide a facile approach to figure out the direction of 2D crystals without complex characterization process, which is valuable for material processing of 2D materials.

References

[1] Joe, M. et al. A comprehensive study of piezomagnetic response in $CrPS_4$ monolayer: mechanical, electronic properties and magnetic ordering under strains. J. Phys. Condens. Matter 29, (2017) 405801.

Figures

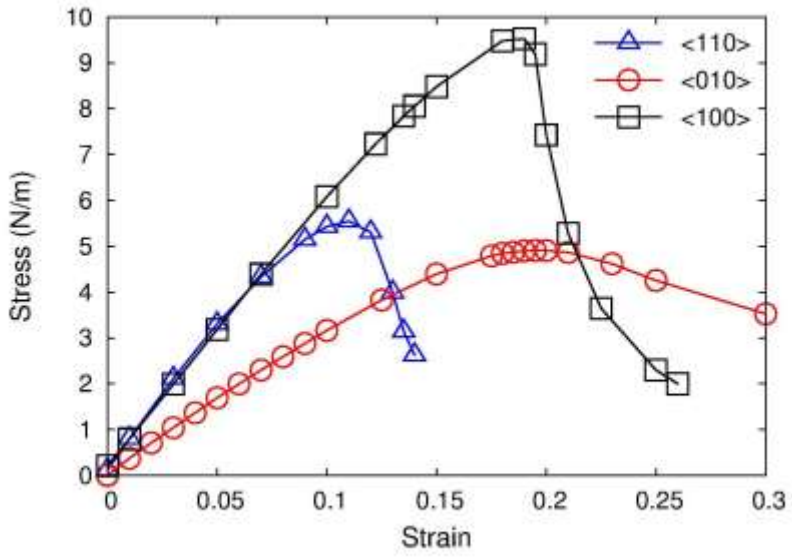

Figure 1: Stress-strain curve of monolayer $CrPS_4$ under different uniaxial directions.