

Li, An, and Morozov Reply: In the preceding Comment [1], Yang *et al.* applied *ab initio* calculations to show that the In–Sb bond rearrangement in twinned InSb leads to the rearranged structure exactly the same as the original twin structure. This results in the identical stress peaks, which is different from our previous results showing that the In–Sb covalent bond rearrangement leads to the gradual ascent of the stress peaks in Ref. [2].

We acknowledge Yang’s comments for correcting our stress output results of nanotwinned InSb [Fig. 1(e) in Ref. [2]]. Figures 1(a) and 1(b) below show our shear loading method and Yang’s shear loading method. In our loading method, each shear strain (α) was applied on the system through simultaneously changing the a axis and c axis with a $\alpha/2$ shear strain. In Yang’s method, the c axis was changed with an α shear strain while the a axis remains

unchanged. Our shear loading method could cause the twin boundary not to be parallel to the x axis, leading to the output stress (σ_{zx}) not representing the stress on the $(111)\langle 112 \rangle$ slip system.

However, as corrected by Yang, the shear stress output with coordinate transformation is similar with that in Yang’s loading method [Fig. 1(c)]. In addition, our calculated structure of nanotwinned InSb after In–Sb bond rearrangement is exactly the same as that calculated by Yang [Figs. 1(d)–1(e)]. This suggests that these two loading methods have no obvious difference in investigating the mechanical behavior of nanotwinned InSb. Importantly, there is still an obvious strength enhancement in nanotwinned InSb (2.65 GPa) than its ideal single crystalline InSb (2.43 GPa), which is consistent with the major conclusions in our Letter [2].

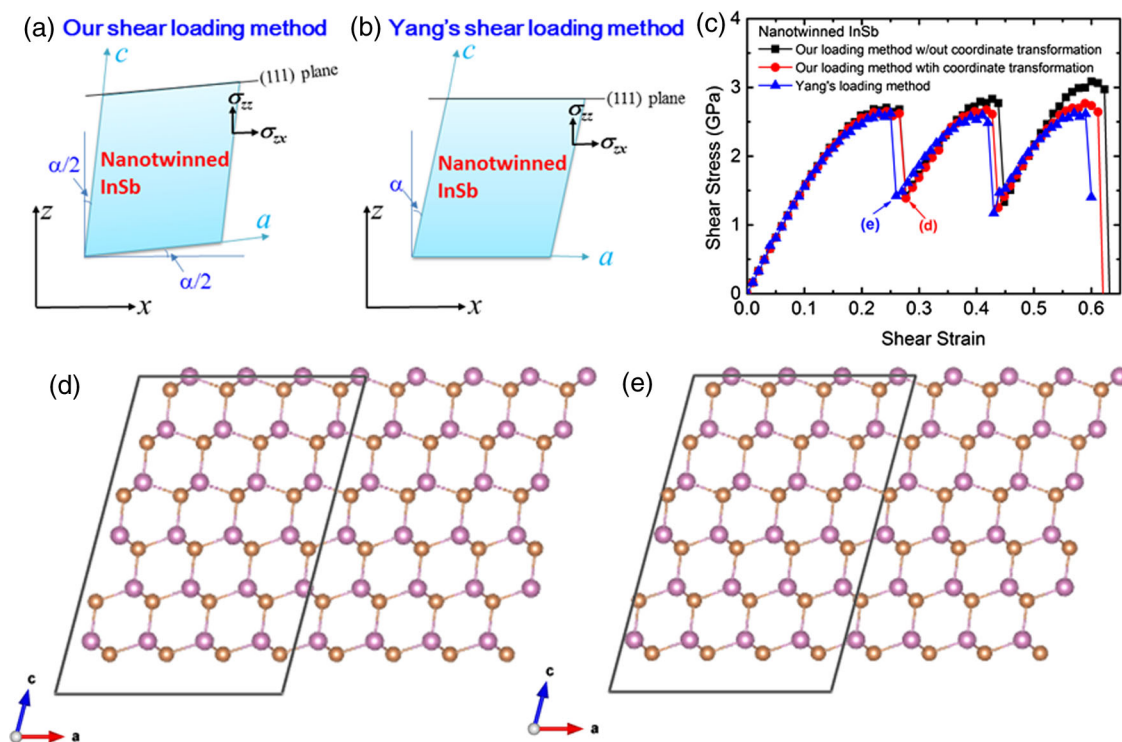


FIG. 1. (a) Our shearing loading method and (b) Yang’s shear loading method. (c) The stress output with and without coordinate transformation in our loading method, and the comparison with that in Yang’s loading method. (d) Our and (e) Yang’s calculated structure of nanotwinned InSb after In–Sb bond rearrangement.

In summary, Yang's work used *ab initio* calculations to study another shear loading method on mechanical behavior of nanotwinned InSb, and there is no obvious difference in stress output and structural deformation. Their work is consistent with the main conclusions and innovations of our previous work [2].


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- [1] B. Yang, X. Peng, C. Huang, Y. Zhao, and T. Fu, preceding Comment, *Phys. Rev. Lett.* **123**, 119601 (2019).
[2] G. Li, S. I. Morozov, Q. Zhang, Q. An, P. Zhai, and G. J. Snyder, *Phys. Rev. Lett.* **119**, 215503 (2017).