Comment on "Enhanced Strength Through Nanotwinning in the Thermoelectric Semiconductor InSb"

In Ref. [1], Li *et al.* used first-principles calculations to show the enhancement of the strength of InSb arising from twin boundaries (TBs). The authors gave the stress-strain (σ-ε) curve of nanotwinned-InSb (nt-InSb) along the $(111)\langle 112\rangle$ slip system. The curve exhibits a distinct zigzag, where the stress peaks ascend gradually. However, the covalent bond rearrangement presented in this Letter obviously contradicts with the gradual ascent of the stress peaks.

To clarify this issue, we reproduce the σ-ε curves of nt-InSb and flawless InSb along the $(111)\langle 112\rangle$ slip system, using the computational models and parameters given in Ref. [1], as shown in Fig. 1(a), where the stress peaks of nt-InSb are $\sigma_1 = 2.62$, $\sigma_2 = 2.59$, and $\sigma_3 = 2.62$ GPa, respectively, which are basically identical, but quite different from the three stress peaks of 2.70, 2.77, and over 3.00 GPa in Ref. [1]. To confirm the rationality of our results, some key structural snapshots of nt-InSb subjected to strains from $\varepsilon_1 = 0.25$ to $\varepsilon_2 = 0.26$ are extracted, as shown in Figs. 1(c) and 1(d), respectively. The atomic arrangement of InSb can be regarded as the typical diamond structure, in which there are two nonequivalent families of (111) planes, with narrowly spaced atomic layers (glide set) and widely spaced atomic layers (shuffle set) [2]. The covalent bond rearrangement is accomplished with the break of bond Sb_1-In_2 and the formation of bond Sb_1-In_3 that occurs on the shuffle-set plane, attributed to that the energy barrier (γ_U) on the shuffle-set plane is lower than that on the glide-set plane. The lower γ_U implies the easier slip path [3,4]. The calculated generalized stacking fault energy (GSFE) curves for InSb along the $(111)\langle 112\rangle$ slip system are shown in Fig. 1(b), where the energy barrier difference ($\Delta\gamma$) is equal to 137 mJ/m^2, which convincingly illustrates why the covalent bond rearrangement should occur on the shuffle-set plane. After the rearrangement of the covalent bonds, the newly formed structure retains the nanotwinned structure, as shown in Fig. 1(d). To confirm the equivalence between the new structure and the original one, we unload the stress from ε_2 by reducing the applied strain until $\sigma = 0$, and find that the relaxed

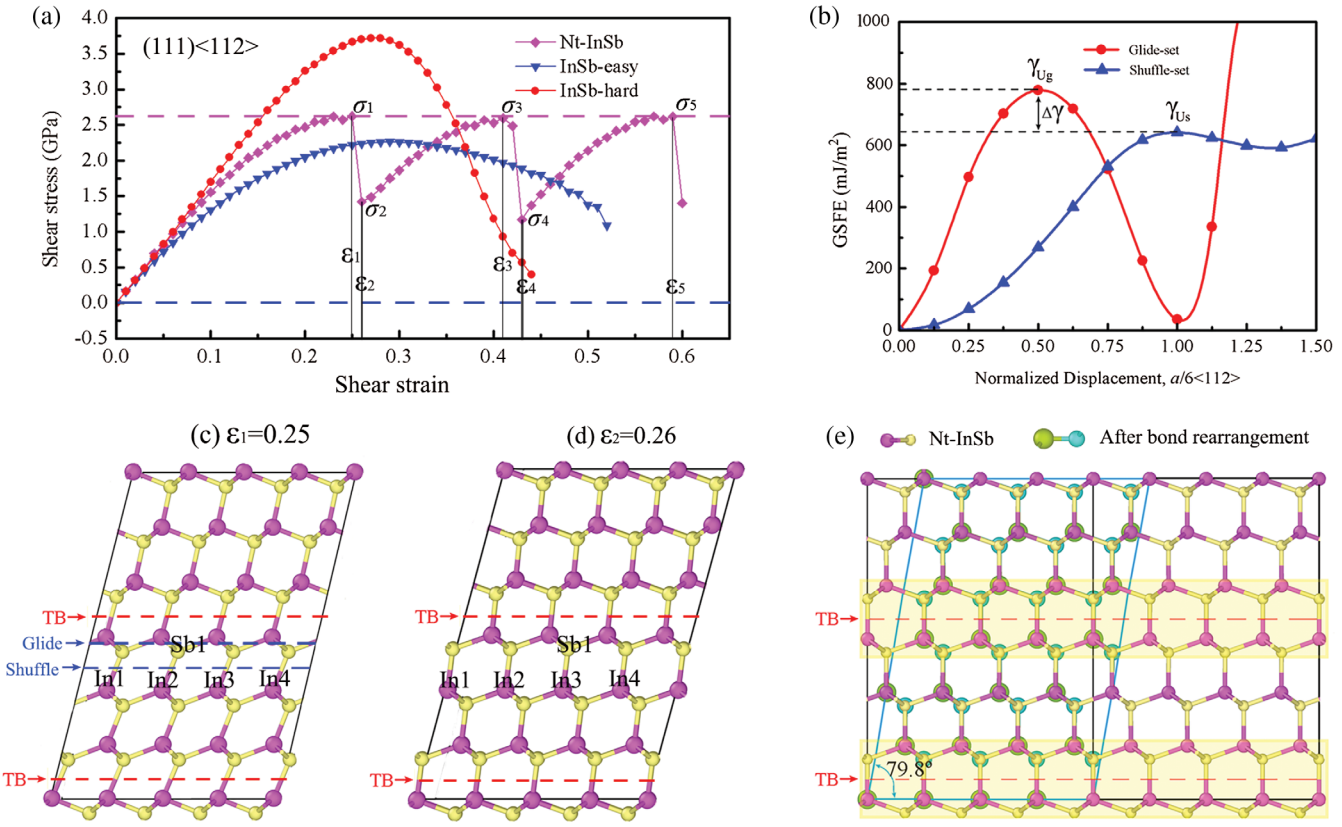

FIG. 1. (a) Comparison between the σ-ε curve of nt-InSb under pure shear and that of flawless InSb sheared along the easy $(111)[11\bar{2}]$ and hard $(111)[\bar{1}\,\bar{1}\,2]$ directions. (b) Calculated GSFE curves of InSb along the $(111)\langle 112\rangle$ slip system, with γ_{Ug} and γ_{Us} denoting the energy barrier on glide-set and shuffle-set planes, respectively. (c) and (d) Structural snapshots of nt-InSb under shear at $\varepsilon_1 = 0.25$ and $\varepsilon_2 = 0.26$. (e) Comparison between the atomic structure of the original nt-InSb and nt-InSb unloaded from $\varepsilon_2 = 0.26$ and relaxed; with red dashed lines representing twin boundaries.

unloaded atomic structure is exactly consistent with that of the original nt-InSb. Figure 1(e) shows the comparison between the atomic structure of the original nt-InSb and that of the nt-InSb after being strained, unloaded, and relaxed, where the positions of the atoms in the two structures coincide exactly, which implies that the stress peaks of nt-InSb should be basically identical, rather than gradually increase, as described in Ref. [1].

We also explore the reasons for incorrect stress output in Ref. [1], and find that it should be attributed to the mishandling of the rotation of the deformed configuration. Because of it, the discussion related to the enhancement of strength would no longer make sense.

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