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The role of $\{100\}_r$-type twinning in Structural Relaxation of B_4C Fivefold Twinned Nanowires

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$\{100\}_r$-type twinned planes formed by the close-packing of boron icosahedral clusters in B_4C play an important role for the formation, growth and structural relaxation of nanowires with nominally fivefold symmetry (r stands for rhombohedral structure). We demonstrate that the {100}r-type twinned plane plays a crucial role in the incoherent structural relaxation of B_4C fivefold twinned nanowires (FTNWs) which exhibits a larger angular mismatch about $5°$. It does so by forming microtwin lamella which terminates at dislocation arrays forming a small angle grain boundary. We can show that this is energetically favored configuration for large diameter nanowires under study.

Figure 1 shows the result of a side-view transmission electron microscopy of a B_4C nanowire. Electron diffraction pattern in Fig. 1(a) can be successfully interpreted as a composite of diffraction patterns from all five crystallites individually labeled as T1-T5 respectively where the twinning systems between them are assumed being $\{100\}_r < 011 >_r$. This is structurally related to the FTNW discovered in boron suboxide. The dark-field (DF) electron microscopy images using the marked diffracted beams in Fig 1(a) show a reasonable correspondence between the diffracting regions and the projection from the proposed cross-section of the nanowire [Fig. 1(b-f)], particularly so for T1, T3 and T4. The patched diffraction contrasts for T2 and T5 may be due to their overlap with the strongly diffracting T3 and T4 respectively. The first evidence suggesting an incoherent structural relaxation mechanism to relieving the resulting stress is the observation of four distinct parallel dark lines along the growth direction in the DF image of T3 [Fig. 1(d)]. Filterd HRTEM [in the lower part of Fig. 1(g)] revels that these dark lines correspond to some $\{100\}_r$ –type microtwins (MTs) lamella with almost regualr spacing. The diffraction index and the crystallography analysis suggest that there is a negative angular mismatch of $5°$ for the unrelaxed B_4C FTNW [1] in contrst to the B_6O FTNWs [2] with smaller pasitive angular mismatch [Fig. 1(g)].

The experimental result may be understood in terms of a defect structural model proposed in Fig. 2(a). It consists of a star-disclination core and a stress-reliving SAGB in the middle of T3 augmented by a set of intersecting MT lamella pairs (SAGB+MT). By drawing Burgers circuit around a dislocation core in the SAGB+MT model and SAGB model respectively, we can show that the introducing of microtwin lamella pairs reduces the elastic energy of the dislocation core corresponding to the reduction of the effective Burgers vector [Fgi. 2(c) (d)]. The experimental result also surports the SAGB+MT model as shown in Fig. 2(f). The energetics of such a defect model can be compared with other alternatives quantitatively [Fgi. 2(g)]. It is clear that the SAGB+MT model is energetically more favorable for FTNWs with a large radius and a large angular mismatch. This is consistent with the lack of such microtwin defects in boron suboxide multiply twinned nanowires with an even larger radius of 40 nm [2], another superhard materials but with almost zero angular mismatch. Our model is consistent with the defect structure observed in multiply twinned nanoparticles of silicon [3] and germanium [4] where the role of microtwins is taken up by stacking faults.

We hope that our detailed relaxation model provide a realistic starting point to take these into account in understanding of the physical properties of incoherently relaxed nanowire structure.

References
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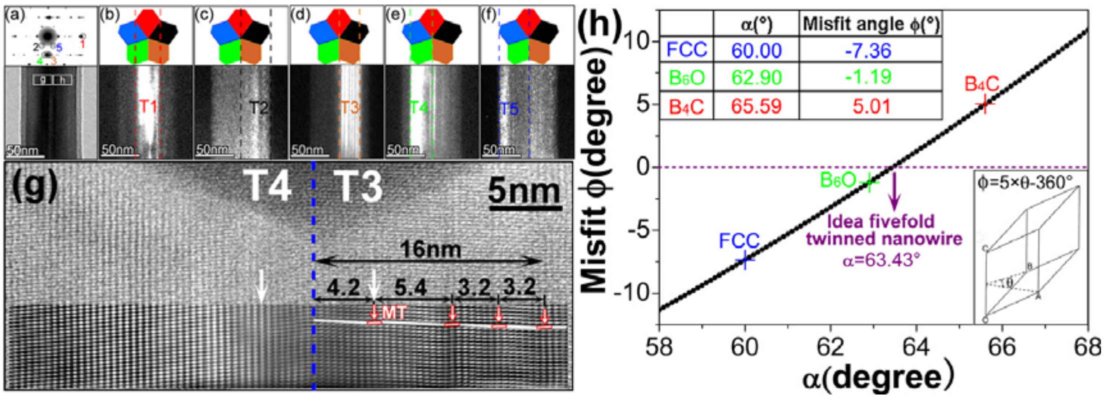

FIG. 1. (a) The bright field image and the corresponding diffraction patterns of a B_4C fivefold twinned nanowire. (b-f) The dark field (DF) images of five crystallites aligned with the corresponding segments in the cross-sectional model. (g) The HR image of the same regions shown in (a); the dashed blue line indicates the interface between T3 and T4. The Fourier filtered images are also displayed in the lower part of (g), the $(112)_r$ planes of T3 and the microtwins (MTs) are marked by the zigzag solid line. (h) The relationship between the misfit angles (ϕ) and the dihedral angle (α) of the rhombohedral unit cell.

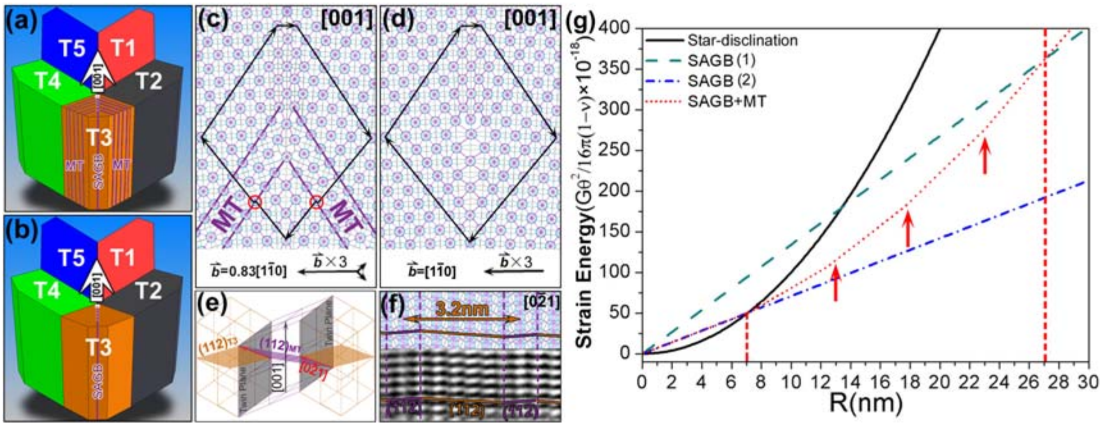

FIG. 2. (a-b) The schematics of the two structural relaxation models of the B_4C fivefold twinned nanowire: SAGB+MT and SAGB respectively; (c-d) The cross-sectional view of the atomic structure of the dislocation cores, respectively, together with the effective Burgers circuits and the unbalanced displacements drawn by black arrowed lines. (e) The relationship between the nanowire axis (the $[001]_r$ direction) and the side view observation direction (the $[0\bar{2}1]_r$, direction). (f) The direct comparison of HRTEM observation with the projecting atomic structure of the SAGB+MT model. (g) The internal strain energies as a function of the nanowire radius for the star-disclination model, the pure small angle grain boundary model (SAGB1) and the SAGB+MT model respectively (SAGB2 did not include the additional twin boundary energy). The arrows indicate the expected positions of the edge dislocation.