Predictable and Controllable Dual-phase Interfaces in
TiO$_2$ (B)/Anatase Nanofibers

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Supplementary Materials

Calculation procedure with crystallographic model

According to Euler’s theorem dealing with rigid-body rotation, the rotation axis $u$ and angle $\theta$ can be determined by resolving the Euler equation as follows:

$$
\frac{(P_2 - P_1) \times (Q_2 - Q_1)}{(P_2 + P_1) \cdot (Q_2 - Q_1)} = u \tan \frac{\theta}{2}
$$

(A-1)

where $P_1$ and $Q_1$ are the invariant unit vector in real and in reciprocal space, $P_2$ and $Q_2$ are the corresponding invariant unit vector after the Bain deformation. The four vectors are given as follows:

$$
\begin{align*}
P_1 &= b / |b| \\
Q_1 &= [hkl] \\
P_2 &= B \cdot b / |B \cdot b| \\
Q_2 &= Q_1 \cdot B^{-1}
\end{align*}
$$

(A-2)

Here, $b$ is the Burgers vector of an edge dislocation which lies on the habit plane. As the invariant unit vector will not change in both direction and length, the following relationship can be obtained:

$$
\begin{align*}
P_1 \cdot Q_1 &= 0 \\
|P_1| &= |P_2| \\
|Q_1| &= |Q_2|
\end{align*}
$$

(A-3)

As the specific feature of TiO$_2$ (B) crystal structure, the Burgers vectors are chosen to be [$032]_{TB}$, which is the shorter than [$010]_{TB}$. The $P_1$ was expressed to be [13,10,1] in coordinate system.
Under the conditions shown in Equation (A-3), there are
\[
\begin{align*}
13h + 10k + l &= 0 \\
\lambda^2 + k^2 + l^2 &= \frac{h^2}{\eta_1^2} + \frac{k^2}{\eta_2^2} + \frac{l^2}{\eta_3^2}
\end{align*}
\] (A-4)

The value \(\eta_1\), \(\eta_2\) and \(\eta_3\) are the components of Bain matrix along three basal axes. And they are shown as below:
\[
B = \begin{bmatrix}
\eta_1 & 0 & 0 \\
0 & \eta_2 & 0 \\
0 & 0 & \eta_3
\end{bmatrix} = \begin{bmatrix}
[3[711]_{TA}] & 0 & 0 \\
[0011]_{TB}^* & 0 & 0 \\
[1110]_{TB}^* & 0 & 0
\end{bmatrix} = \begin{bmatrix}
1.0409 & 0 & 0 \\
0 & 1.0323 & 0 \\
0 & 0 & 0.8540
\end{bmatrix}
\]

Based on the Equation (A-3) and the values of \(\eta_1\), \(\eta_2\) and \(\eta_3\), the \(Q_1\) was calculated to be \(Q_1 = [0.8117, 1, 0.5521]\). Therefore, the rotation axis \(u\) and angle \(\theta\) can be obtained to be [0.6983, 0.71579, 0.001403] (which is under coordinate system) and \(-4.3^\circ\) by resolving Equation (A-1).

Therefore, the rotation matrix \(R\) can be obtained as blow, when let the unit rotation axis \(u\) as\([p_1, p_2, p_3]\):
\[
R = \begin{bmatrix}
a_{11} & a_{12} & a_{13} \\
a_{21} & a_{22} & a_{23} \\
a_{31} & a_{32} & a_{33}
\end{bmatrix} = \begin{bmatrix}
p_1^2(1 - \cos \theta) + \cos \theta & p_1p_2(1 - \cos \theta) - p_1 \sin \theta & p_1p_3(1 - \cos \theta) + p_2 \sin \theta \\
p_2p_1(1 - \cos \theta) + p_1 \sin \theta & p_2^2(1 - \cos \theta) + \cos \theta & p_2p_3(1 - \cos \theta) - p_1 \sin \theta \\
p_3p_1(1 - \cos \theta) - p_2 \sin \theta & p_3p_2(1 - \cos \theta) + p_1 \sin \theta & p_3^2(1 - \cos \theta) + \cos \theta
\end{bmatrix}
\]

As the total strain matrix can be written as:
\[
A = RB = \begin{bmatrix}
a_{11} & a_{12} & a_{13} \\
a_{21} & a_{22} & a_{23} \\
a_{31} & a_{32} & a_{33}
\end{bmatrix} \begin{bmatrix}
\eta_1 & 0 & 0 \\
0 & \eta_2 & 0 \\
0 & 0 & \eta_3
\end{bmatrix} \] (A-5)

The invariant line can be obtained by setting the eigenvalues \(\lambda\) equal to unity. And the
eigenvalues are the roots of the equation

$$|A - \lambda I| = 0$$  \hspace{1cm} (A-6)$$

From which

$$|A - \lambda I| = |RB - \lambda I| = \lambda^3 - S_1\lambda^2 + S_2\lambda - S_3 = 0$$  \hspace{1cm} (A-7)$$

It is easy to prove that $S_2 - S_1 = S_3 - 1$.

The equation (A-7) has a form of

$$\lambda^3 - S_1\lambda^2 + S_2\lambda - S_3 = (\lambda - 1)[\lambda^2 - (S_1 - 1)\lambda + S_3]$$  \hspace{1cm} (A-8)$$

The eigenvalues are then found to be

$$\begin{cases}
\lambda_1 = 1 \\
\lambda_{2,3} = \frac{S_1 - 1 \pm \sqrt{(S_1 - 1)^2 - 4S_3}}{2}
\end{cases}$$

When $\lambda_1 = 1$, the corresponding eigenvector can be obtained to be $[0.5604, 0.6882, 0.4607]$ under coordinate system. Its corresponding vector under original TiO$_2$ (B) phase system is $[2,13,1]$ in (001) plane, $25.6^\circ$ away from [010].

Table 1 shows all the key elements defined and calculated in the IDE crystallographic model.

<table>
<thead>
<tr>
<th>Elements defined</th>
<th>Original coordinate system (TB)</th>
<th>Reference Cartesian coordinate system</th>
<th>Referred</th>
</tr>
</thead>
<tbody>
<tr>
<td>Non-inclined Line</td>
<td>$P_1 = [032]_{TB}$</td>
<td>$P_1 = [13,10,1]$</td>
<td></td>
</tr>
<tr>
<td>Invariant Normal</td>
<td>$Q_1 = [375]$</td>
<td>$Q_1 = [0.8117,1,0.5521]$</td>
<td></td>
</tr>
<tr>
<td>Rotation Axis</td>
<td>$[1,31,11]_{TB}$</td>
<td>$[0.6983,0.7158,0.0014]$</td>
<td></td>
</tr>
<tr>
<td>Rotation Angle</td>
<td>$-4.3^\circ$</td>
<td>$-4.3^\circ$</td>
<td>Fig. 2(g)</td>
</tr>
<tr>
<td>Invariant Line (Habit Plane)*</td>
<td>$[2,13,1]_{TB}$</td>
<td>$[0.5604,0.6882,0.4607]$</td>
<td></td>
</tr>
<tr>
<td>(Habit Plane)*</td>
<td>$[81\bar{5}]_{TB}$</td>
<td>$[0.3261,0.3280,0.8867]$</td>
<td></td>
</tr>
</tbody>
</table>

The asterisk “*” expresses the planar normal.