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On the Growth Morphology and Crystallography of Epitaxial CdTe/Cu_7Te_4 Interface

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Supplymentary Materials

The detailed NCSL calculation process on the CdTe/Cu_7Te_4 interface

According to the defination of NCSL, the basal vectors of CdTe substrate $\boldsymbol{R}_{S1}$, $\boldsymbol{R}_{S2}$ and $\boldsymbol{R}_{F1}$, $\boldsymbol{R}_{F2}$ can be written as:

$$R_{S1} = a_1\begin{bmatrix}1\\0\end{bmatrix},\ R_{S2} = \frac{\sqrt{2}}{2}a_1\begin{bmatrix}0\\1\end{bmatrix} \qquad \text{(S1)}$$

$$R_{F1} = c\begin{bmatrix}1\\0\end{bmatrix},\ R_{F2} = \frac{\sqrt{3}}{2}a_2\begin{bmatrix}0\\1\end{bmatrix} \qquad \text{(S2)}$$

Here, a_1 and a_2, c represents the lattice parameter of CdTe and Cu_7Te_4 respectively.

After the rotation process, the vectors $\boldsymbol{R}_{RF1}$ and $\boldsymbol{R}_{RF2}$ can also be obtained:

$$\left(R_{RF1}, R_{RF2}\right) = (Z/\theta)\left(R_{F1}, R_{F2}\right) \tag{S3}$$

Here, (Z/θ) represents the rotation matrix which can be expressed as:

$$(Z/\theta) = \begin{bmatrix} cos\theta & -\,sin\theta \\ sin\theta & cos\theta \end{bmatrix} \tag{S4}$$

In this case, the Eq. (S3) can be written as:

$$\left(R_{RF1}, R_{RF2}\right) = \begin{bmatrix} cos\theta & -\,sin\theta \\ sin\theta & cos\theta \end{bmatrix}\begin{bmatrix} c & 0 \\ 0 & \frac{\sqrt{3}}{2}a_2 \end{bmatrix} = \begin{bmatrix} ccos\theta & -\frac{\sqrt{3}}{2}a_2 sin\theta \\ csin\theta & \frac{\sqrt{3}}{2}a_2 cos\theta \end{bmatrix} \tag{S5}$$

Therefore,

$$R_{RF1} = c\begin{bmatrix} cos\theta \\ sin\theta \end{bmatrix}, R_{RF2} = \frac{\sqrt{3}}{2}a_2\begin{bmatrix} -\,sin\theta \\ cos\theta \end{bmatrix} \tag{S6}$$

In this case, the NCSL basal vectors $\boldsymbol{V_1}$ and $\boldsymbol{V_2}$ can be expressed as:

$$V_1 = mR_{S1} + nR_{S2} = a_1\begin{bmatrix} m \\ 0 \end{bmatrix} + \frac{\sqrt{2}}{2}a_1\begin{bmatrix} 0 \\ n \end{bmatrix} = a_1\begin{bmatrix} m \\ \frac{\sqrt{2}}{2}n \end{bmatrix} \tag{S7}$$

$$V_2 = pR_{RF1} + qR_{RF2} = pc\begin{bmatrix} cos\theta \\ sin\theta \end{bmatrix} + \frac{\sqrt{3}}{2}qa_2\begin{bmatrix} -\,sin\theta \\ cos\theta \end{bmatrix} = \begin{bmatrix} pccos\theta - \frac{\sqrt{3}}{2}qa_2 sin\theta \\ pcsin\theta + \frac{\sqrt{3}}{2}qa_2 cos\theta \end{bmatrix} \tag{S8}$$

Here, m, n, p and q are all integers. According to the defination of NCSL, $\boldsymbol{V_1}$ and $\boldsymbol{V_2}$ should be equal, the 2 vectors must have the same vector module and parallel to each other. Therefore, combine the Eq. (S7) and (S8), the following equation can be obtained:

$$\begin{cases} ma_1 = pccos\theta - \frac{\sqrt{3}}{2}qa_2 sin\theta \\ \frac{\sqrt{2}}{2}na_1 = pcsin\theta + \frac{\sqrt{3}}{2}qa_2 cos\theta \end{cases} \tag{S9}$$

From Eq. (S9), the expressions of tanθ, Σ and the relationship between the 4 integers can be obtained accordingly:

$$\begin{cases} m^2a_1^2 + \frac{1}{2}n^2a_1^2 = p^2c^2 + \frac{3}{4}q^2a_2^2 \\ tan\theta = \frac{2\sqrt{2}npc - 2\sqrt{3}mqa_2}{4mpc + \sqrt{6}nqa_2} \\ \Sigma = \frac{V_{Super}}{V_{Unit}} = \frac{4p^2c^2 + 3q^2a_2^2}{2\sqrt{3}a_2c} \end{cases} \quad \text{(S10)}$$

According to the TEM results in Fig. 2, the parallel relationship of $(1\bar{1}1)_{CdTe}//(0001)_{Cu_7Te_4}$ can be obtained. In addition, it is also noticed that the interplanar distance of $(0001)_{Cu_7Te_4}$ (0.7211 nm) is very close to that of $(01\bar{1}0)_{Cu_7Te_4}$ (0.7218 nm). This means that the established Cu_7Te_4 unit cell is similar to square. To simplify the calculation, the following relations can be set:

$$\begin{cases} \frac{\sqrt{3}}{3}a_1 = \frac{1}{2}c \\ c = \frac{\sqrt{3}}{2}a_2 \end{cases} \quad \text{(S11)}$$

In this case, Eq. (S10) can be simplified to be:

$$\begin{cases} \frac{3}{4}m^2 + \frac{3}{8}n^2 = p^2 + q^2 \\ tan\theta = \frac{\sqrt{2}np - 2mq}{2mp + \sqrt{2}nq} \\ \Sigma = \frac{V_{Super}}{V_{Unit}} = p^2 + q^2 \end{cases} \quad \text{(S12)}$$

Under the principle that the value of the 4 integers should be as small as possible, the calculation results are summarized in Table S1. The rotation angle of ±54.74° and ±35.26° refer to the variant 1 and 2 of Cu_7Te_4 respectively. The same Σ values suggest the equivalent status of the COR obtained by applying the rotation along the 4 rotation angles.

Table S1 The calculation results of the $CdTe/Cu_7Te_4$ interface

m	n	p	q	$\tan\theta$	θ	Σ
2	4	3	0	$\sqrt{2}$	54.74°	9
-2	4	3	0	$-\sqrt{2}$	-54.74°	9
2	4	0	3	$-\frac{\sqrt{2}}{2}$	-35.26°	9
-2	4	0	3	$\frac{\sqrt{2}}{2}$	35.26°	9