Analysis of the period of the moire supercell on vdW heterostructures

Shin Yasuda
University of Toyama

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1 Introduction

This paper is aimed to deduce the general formula of the period of the moire supercell on vdW heterostructures.

2 setting and ingredients

Our targets are the vdW heterostructures. That's a class of material where two or more layers by different atomic species are stacked rotationally aligned or twisted. What is interesting is that if there is any lattice mismatch or rotation of a layer in two-layered material, it should have a long-period structure called moire supercell. We would like to calculate how is it expressed and applied to numerical approach in X-ray Photoelectron diffraction.
The ingredients needed to catch up the following calculation flow are easy-peasy. Firstly, we have the rotation matrix:

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}, \tag{1}$$

where we think the anticlockwise rotation in the whole. Finally, we treat only the hexagonal structures with lattice vectors as follows:

$$\boldsymbol{a}_1 = \begin{pmatrix} a \\ 0 \end{pmatrix} \ \boldsymbol{a}_2 = \frac{a}{2}\begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix}, \tag{2}$$

where we denote the lattice constant as a.

3 Deduction

Here we consider the case in which two hetero atomic layers are stacked and the top layer is rotated along z-axis, stacking direction by θ anticlockwise. The case where we see only lattice mismatch between the two layers rotationally aligned can be understood in the limit of $\theta \to 0$. We start with getting the reciprocal vector of each layer:

$$\begin{aligned} \boldsymbol{b}_1 &= \frac{2\pi}{a}\begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \end{pmatrix} \ \boldsymbol{b}_2 = \frac{2\pi}{a}\begin{pmatrix} 0 \\ \frac{2}{\sqrt{3}} \end{pmatrix} \\ \boldsymbol{b}_1^{'} &= \frac{2\pi}{a^{'}}\begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \end{pmatrix} \ \boldsymbol{b}_2^{'} = \frac{2\pi}{a^{'}}\begin{pmatrix} 0 \\ \frac{2}{\sqrt{3}} \end{pmatrix} \end{aligned} \tag{3}$$

where a is the lattice constant of the bottom layer and $a^{'}$ is that of the top layer. If the top layer is rotated in our manner, its reciprocal vectors change to:

$$\boldsymbol{b}_j^{'} \to R(\theta)(1+\epsilon)\boldsymbol{b}_j \ \left(1+\epsilon = \frac{a^{'}}{a}\right) \tag{4}$$

We rely on a formula introduced in [1] that the reciprocal vectors corresponding to the moire supercell should be:

$$\boldsymbol{G}_j^M = \boldsymbol{b}_j - \boldsymbol{b}_j^{'} \tag{5}$$

This phenomenon is physically related to beats, which are commonly observed in waves. When two waves with different periods (reciprocal lattices) overlap, a new long-period wave (moiré superlattice) emerges and is observed as a beat.

To be honest, we have to evaluate $\boldsymbol{G}_j^M$ as the following flow:

$$\boldsymbol{G}_1^M = \boldsymbol{b}_1 - R(\theta)(1+\epsilon)^{-1}\boldsymbol{b}_1 = \frac{2\pi}{a}\begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \\ 0 \end{pmatrix} - \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}(1+\epsilon)^{-1}\frac{2\pi}{a}\begin{pmatrix} 0 \\ \frac{2}{\sqrt{3}} \\ 0 \end{pmatrix}$$

$$= \frac{2\pi}{a}\begin{pmatrix} 1 - \frac{1}{1+\epsilon}\left(\cos\theta + \frac{1}{\sqrt{3}}\sin\theta\right) \\ -\frac{1}{\sqrt{3}} - \frac{1}{1+\epsilon}\left(\sin\theta - \frac{1}{\sqrt{3}}\cos\theta\right) \end{pmatrix} \tag{6}$$

$$\boldsymbol{G}_2^M = \boldsymbol{b}_2 - R(\theta)(1+\epsilon)^{-1}\boldsymbol{b}_2 = \frac{2\pi}{a}\begin{pmatrix} \frac{2\sin\theta}{\sqrt{3}(1+\epsilon)} \\ \frac{2}{\sqrt{3}} - \frac{2\cos\theta}{\sqrt{3}(1+\epsilon)} \end{pmatrix} \tag{7}$$

This is interpreted as the beat phenomenon as two periods of $\boldsymbol{b}_j$ and $\boldsymbol{b}_j^{'}$ lead to a new and longer one that we're trying to get. Actually, we have to go back to the real space, i,e,. identifying coefficients of the moire supercell lattice vectors is needed:

$$\boldsymbol{L}_j^M = l_j^x\begin{pmatrix} 1 \\ 0 \end{pmatrix} + l_j^y\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} l_j^x \\ l_j^y \end{pmatrix} \tag{8}$$

Here, we have two unknown parameters to be determined for each index, j. To accomplish that task, the following relations are useful:

$$\boldsymbol{L}_i^M \cdot \boldsymbol{G}_j^M = 2\pi\delta_{ij} \tag{9}$$

On the date of the first writing, I am going to determine l_1^x and l_1^y. We pick up the following constraints:

$$\boldsymbol{L}_1^M \cdot \boldsymbol{G}_1^M = 2\pi \tag{10}$$

$$\boldsymbol{L}_1^M \cdot \boldsymbol{G}_2^M = 0 \tag{11}$$

We begin with Eq11:

$$\boldsymbol{L}_1^M \cdot \boldsymbol{G}_2^M = \begin{pmatrix} l_1^x \\ l_1^y \end{pmatrix} \cdot \frac{2\pi}{a}\begin{pmatrix} \frac{2\sin\theta}{\sqrt{3}(1+\epsilon)} \\ \frac{2}{\sqrt{3}} - \frac{2\cos\theta}{\sqrt{3}(1+\epsilon)} \end{pmatrix}$$

$$= \frac{2\pi}{a}\left\{\left(\frac{1}{1+\epsilon}\frac{2}{\sqrt{3}}\sin\theta\right)l_1^x + \left(\frac{2}{\sqrt{3}} - \frac{1}{1+\epsilon}\frac{2}{\sqrt{3}}\cos\theta\right)l_1^y\right\} = 0$$

$$l_1^x = \frac{\cos\theta - (1+\epsilon)}{\sin\theta}l_1^y \tag{12}$$

The next is:

$$\boldsymbol{L}_1^M \cdot \boldsymbol{G}_1^M = \begin{pmatrix} l_1^x \\ l_1^y \end{pmatrix} \cdot \frac{2\pi}{a}\begin{pmatrix} 1 - \frac{1}{1+\epsilon}\left(\cos\theta + \frac{1}{\sqrt{3}}\sin\theta\right) \\ -\frac{1}{\sqrt{3}} - \frac{1}{1+\epsilon}\left(\sin\theta - \frac{1}{\sqrt{3}}\cos\theta\right) \end{pmatrix}$$

$$= \frac{2\pi}{a}\left[\left\{1 - \frac{1}{1+\epsilon}\left(\cos\theta + \frac{1}{\sqrt{3}}\right)\right\}l_1^x - \left\{\frac{1}{\sqrt{3}} + \frac{1}{1+\epsilon}\left(\sin\theta - \frac{1}{\sqrt{3}}\cos\theta\right)\right\}l_1^y\right]$$

$$= 2\pi \tag{13}$$

What we are going to do is to insert Eq12 into Eq13 to see t_1^y:

$$
\begin{aligned}
l_1^y &= a\frac{(1+\epsilon)\sin\theta}{2(1+\epsilon)\cos\theta-(1+\epsilon)^2-1}\\
l_1^x &= a\frac{(1+\epsilon)\cos\theta-(1+\epsilon)^2}{2(1+\epsilon)\cos\theta-(1+\epsilon)^2-1}
\end{aligned}
\tag{14}
$$

To be sure, we take the length of $\boldsymbol{L}_1^M$ given Eq14:

$$
\begin{aligned}
\left|\boldsymbol{L}_1^M\right|^2 &= l_1^{x2}+l_1^{x2} = a^2\frac{(1+\epsilon)^2}{1-2\cos\theta(1+\epsilon)+(1+\epsilon)^2}\\
\left|\boldsymbol{L}_1^M\right| &= a\frac{1}{\sqrt{1+\frac{1}{(1+\epsilon)^2}-2\frac{1}{1+\epsilon}\cos\theta}}
\end{aligned}
\tag{15}
$$

If putting $1+\epsilon=\frac{a'}{a}$, we can derive a formula given in [1].
I refer to just results for l_2^x and l_2^y:

$$
\begin{aligned}
l_2^x &= a\frac{(1+\epsilon)+\left(\sqrt{3}\sin\theta-\cos\theta\right)}{2\left\{\frac{1}{1+\epsilon}-2\cos\theta+(1+\epsilon)\right\}}\\
l_2^y &= a\frac{\sqrt{3}(1+\epsilon)-\left(\sqrt{3}\cos\theta+\sin\theta\right)}{2\left\{\frac{1}{1+\epsilon}-2\cos\theta+(1+\epsilon)\right\}}
\end{aligned}
\tag{16}
$$

I just simply checked that these ones satisfy the length condition of the period, $\boldsymbol{L}_2^M$.

References

[1] Japanese book