THEORETICAL PREDICTION OF Sb_2Se_3 GROWTH MORPHOLOGY AND ORIENTATION ON MUSCOVITE MICA SUBSTRATES

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Ever since the first demonstration in 2004, van der Waals heterostructures have received considerable attention due to their unique interlayer coupling and optoelectronic properties. Therefore, such heterostructures can benefit the performance of photodetectors, solar cells or other optoelectronic devices by reducing surface recombination velocity. Sb_2Se_3 is a quasi-one-dimensional material that can form van der Waals heterostructures on other low dimensional or three-dimensional substrates and has been shown to exhibit excellent optoelectronic properties [1, 2]. However, despite few experimental works, the growth mechanism of Sb_2Se_3 on low dimensional substrates is elusive.

Under equilibrium conditions, the growth of low dimensional materials is governed by van der Waals epitaxy. As in classical epitaxy, the growing layer adopts specific orientation to minimize lattice mismatch. The structure of Sb_2Se_3 resembles that of the molecular crystal, therefore the epitaxial relationship on the specific substrate can be estimated through relatively simple algorithm [3]. Therefore, in this work, we aim to predict the orientation of low dimensional materials grown on the specific substrate.

As a case study, we chose to examine epitaxial relation of Sb_2Se_3 and muscovite mica. The determination of the optimum overlayer orientation was accomplished using a simple geometric lattice misfit modelling algorithm that calculates a "dimensionless potential":

$$\frac{V}{V_0} = \left(1 - \frac{\sin(M\pi p_x)\sin(N\pi q_x)}{2MN\sin(\pi p_x)\sin(\pi q_x)} - \frac{\sin(M\pi q_y)\sin(N\pi p_y)}{2MN\sin(\pi q_y)\sin(\pi p_y)}\right); \quad (1)$$

Here the integer numbers M and N define the size of the overlayer, and the values of $p_{x,y}$ and $q_{x,y}$ are defined by a transformation matrix that relates the overlayer lattice vectors $b_{1,2}$ to the lattice vectors of the substrate $a_{1,2}$ [3]. For muscovite mica substrate, the values were taken $a_1=5.18Å$ and $a_2=8.99Å$ with a perpendicular angle, and for Sb_2Se_3 various orientations of the layers and vectors' $b_{1,2}$ lengths were taken for the calculations.

Out of 10 tested planes with miller indices of (hk0), where h varied in 1 to 3 and k in 1 to 5 range, the (120) indicated the point-on-line coincidence at azimuthal angle at θ~90 and 270 deg. A fair agreement was found with experimental results available in the literature. The existence of lattice coincidence verify that molecular crystal lattice misfit modelling algorithm can be suitable for prediction of Sb_2Se_3 morphology and orientation, and could be helpful in van der Waals epitaxial growth of 1D/2D p-n heterostructures optimization and selection of the substrates.

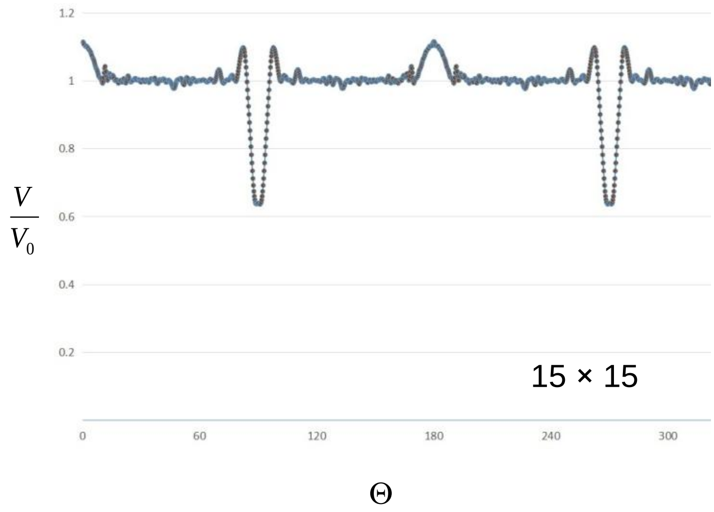

Fig. 1. Dependence of V/V_0 on azimuthal angle Θ for the (120) orientation for Sb_2Se_3 layer with $b_1=3.962Å$, $b_2=26.051Å$ on muscovite mica substrate with $a_1=5.18Å$ and $a_2=8.99Å$. Overlayer size M×N for the calculation is 15×15.

[1] Sun, G., Li, B., Li, J. et al. Nano Res. (2019) 12: 1139. https://doi.org/10.1007/s12274-019-2364-1
[2] Ma Z, Chai S, Feng Q, Li L, Li X, Huang L, Liu D, Sun J, Jiang R, Zhai T, Xu H. ,Small. 2019 Mar;15(9):e1805307. doi:10.1002/smll.201805307
[3] Julie A. Last, Daniel E. Hooks, Andrew C. Hillier, and Michael D. Ward, *The Physicochemical Origins of Coincident Epitaxy in Molecular Overlayers: Lattice Modeling vs Potential Energy Calculations*, J. Phys. Chem. B **1999**, 103, 6723-6733 (1999)