Epitaxial Growth of Monolayer MoS₂ on SrTiO₃ Single Crystal Substrates

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When monolayer molybdenum disulphide (MoS_2) crystals are grown on amorphous substrates such as SiO₂, they are randomly-oriented. The crystal shapes are usually equilateral triangles if grown in a sulphur-rich atmosphere, to minimise the total edge energy [1]. When MoS₂ is grown on crystalline substrates, the shapes and orientations are also influenced by their interaction with the substrate [2-4]. In this work, we grow MoS_2 on three different surface terminations of the single crystal substrate strontium titanate (SrTiO₃) by chemical vapour deposition (CVD), to study the effects of substrate crystallinity on epitaxy. On SrTiO₃(111), they grow into equilateral triangles with two main orientations, in which they align their $<\overline{1}2\overline{1}0>$ -type directions (i.e., edge directions) with the $<\overline{1}10>$ -type (i.e. the close-packed) directions on SrTiO₃ because of coincidence epitaxy. On SrTiO₃(110), the MoS₂ crystals tend to align $<\overline{1}2\overline{1}0>$ with both $<\overline{1}10>$ and $<1\overline{1}\overline{2}>$ on SrTiO₃ as these both provide favourable coincidence lattice registry. This distorts the crystal shapes and hence introduces an additional strain detectable by photoluminescence (PL). When triangular MoS₂ crystals are grown on SrTiO₃(001), they also show a preference to align their edges with $<\overline{110}>$ on SrTiO₃. These observations can be explained by interfacial van der Waals (vdW) bonding between MoS₂ and SrTiO₃, which fluctuates as the MoS₂ nuclei rotate on the substrate surface because the level of lattice registry varies at different orientations. We speculate that the vdW interactions get noticeably enhanced when the two lattices show maximum commensuration, at the experimentally observed orientations. Therefore, a key finding of this paper is the vdW interaction between MoS₂ and SrTiO₃ substrates, which powerfully steers the supported crystal shapes and orientations as determined by the epitaxial relations.



Figure 1: SEM images of monolayer MoS_2 (if not otherwise labelled) on (a) $SrTiO_3(111)$, (b) $SrTiO_3(110)$, and (c) $SrTiO_3(001)$. The insets show the substrate lattices, and the preferred MoS_2 crystal orientations are drawn as blue schematic triangles.

References:

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