Electronic Supporting Information (ESI)

Epitaxial growth of few-layer $MoS_2(0001)$ on $FeS_2\{100\}$

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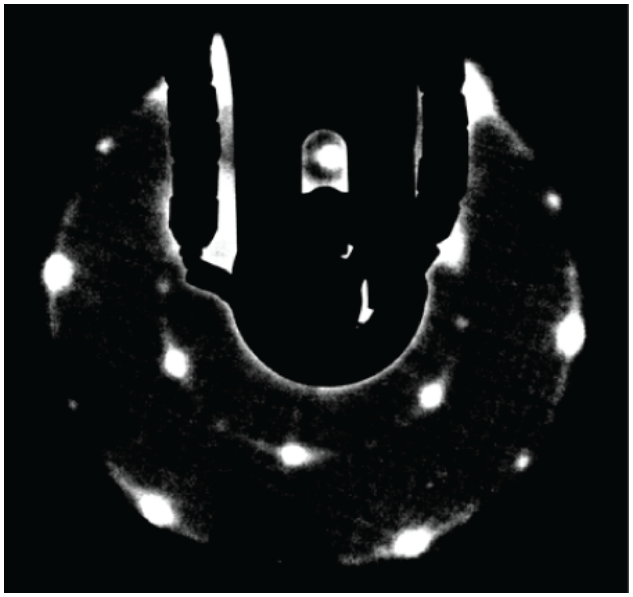

Fig. S1 Digitally enhanced LEED pattern corresponding to 12 min deposition of Mo on $FeS_2\{100\}$ (same data as Fig. 2d in the main text). The 'flatten' filter and 'best fit' histogram equalisation of the Image Pro Plus software package (Media Cybernetics) have been applied to even out the diffuse background intensity and emphasise the low-intensity spots of the secondary (30°-rotated) pattern relative to the main pattern.

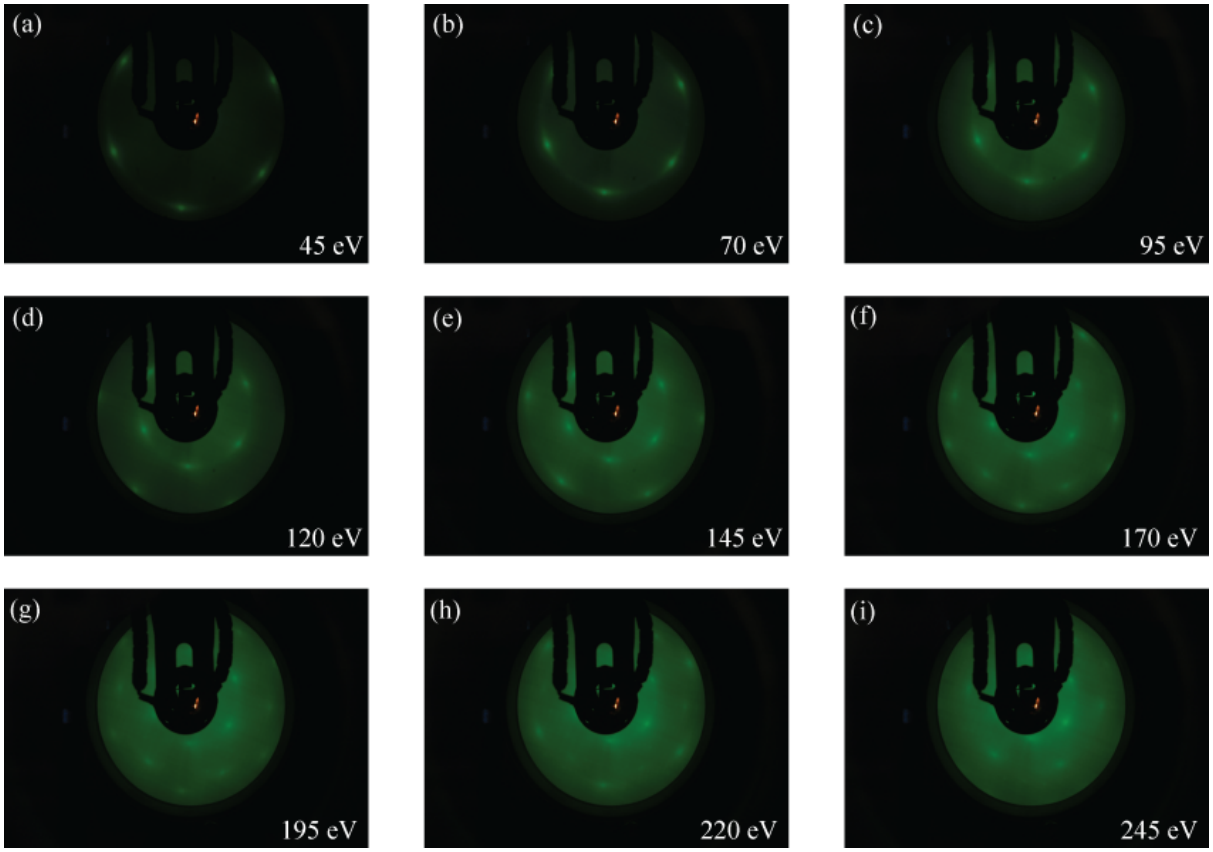

Fig. S2 Series of LEED images, taken at different energies, corresponding to 12 min deposition of Mo on $FeS_2\{100\}$. 6-fold rotational symmetry is apparent in all rings of spots at all energies (see text).

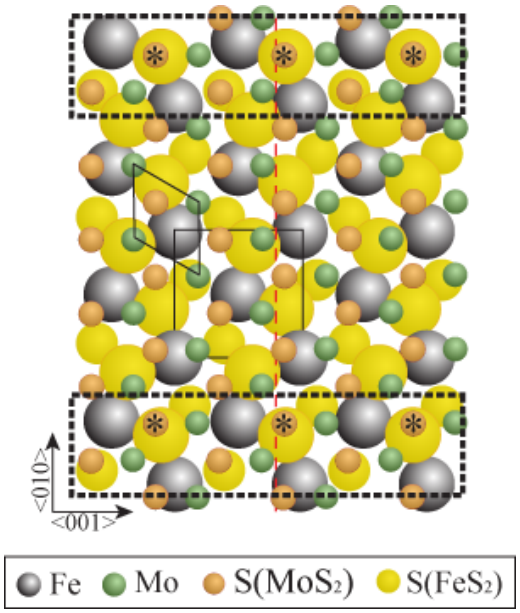

Fig. S3 Approximate lattice match obtained by laying $MoS_2(0001)$ surface structure on top of $FeS_2\{100\}$ at one of the two possible orientations determined by the secondary hexagonal LEED pattern. Notations are equivalent to Fig. 4 in the main text.

Evaluation of MoS_2 film thickness based on calculated electron attenuation lengths

In the main text, we asserted that the MoS_2 overlayer was most likely two trilayers thick. This was based on the almost complete disappearance of the (1×1) LEED pattern of the FeS_2{100} substrate, and the attenuation of the Fe/S Auger peak height ratio to below 10% of its initial value, with a clear break of slope at 9 mins Mo deposition. Electron attenuation lengths in solid materials are known to exhibit a broad minimum in the kinetic energy range applicable to our LEED and AES measurements, such that the attenuation length can be taken as being of the order 1 nm or less in our data.

To quantify this further, we have used the NIST Electron Inelastic Mean Free Path Database[1] to obtain a specific value of the inelastic mean free path (imfp) for electrons travelling in MoS_2. Using values of 5.06 g cm^{-3} for the density of MoS_2, 18 valence electrons per 'molecule', and a band gap (for bulk MoS_2) of 1.2 eV, and using the predictive formula TPP-2M of Tanuma, Powell and Penn (see program documentation), a value of 5.82 Å is obtained for 150 eV electrons in MoS_2, using the NIST program. This value is very comparable with the 6.148 Å layer spacing of successive S-Mo-S trilayers in bulk MoS_2. This would suggest that the signal would attenuate to $1/e$ of its initial value in passing through a single trilayer, and to $1/e^2$ of its initial value in passing through two trilayers.

The formulation does, however, assume an isotropic, homogeneous material, whereas MoS_2 is layered, and thus is neither isotropic nor homogeneous. In addition, in this case a small number of MoS_2(0001) trilayers is epitaxed to FeS_2{100} to make a heterogeneous structure. It is nevertheless reasonable to argue that electrons traversing S-Mo-S trilayers are attenuated primarily in the electron-dense region of the trilayer, rather than in the relatively electron-poor regions between the trilayers. One can then assert that electrons emerging from the outermost FeS_2 layer would attenuate by $1/e$ in passing through a single trilayer, or by $1/e^2$ in passing through two trilayers. Given the degree of attenuation evidenced in the LEED and AES data, two trilayers seems to be the most likely film thickness.

Reference:

1. C. J. Powell and A. Jablonski, *NIST Electron Inelastic-Mean-Free-Path Database* – Version 1.2, National Institute of Standards and Technology, Gaithersburg, MD (2010). [Available online at www.nist.gov/srd/nist71.cfm]