Experimental determination of thermal expansion of natural MoS_2

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Molybdenite (MoS_2) is one of the most widely used materials of the transition metal dichalcogenides (TMDs) family, in part due to its availability in natural form. Recently, there has been renewed interest in this compound as alternative two-dimensional (2D) material beyond graphene. A key aspect of MoS_2 is its easily tunable band gap, whose value is strictly correlated with the thickness and the strain of the crystal. The temperature dependence of the MoS_2 constant lattice is crucial for its integration into different devices in optoelectronics, nanoelectronics and sensors among others. The performance of the aforementioned devices can be precluded because of the expansion induced by the operating temperature of the devices.

We report helium diffraction from natural MoS_2 single crystal and its thermal expansion. The high quality of the samples studied lead to the appearance of sharp and intense in-plane and out-of-plane diffraction peaks, with unusually low background. The pronounced out-of-plane features observed confirm the high corrugation of the 2D surface unit cell.

The observation of diffraction features along the two main high symmetry directions allows determining the in-plane surface lattice constant with high accuracy. The measured lattice constant along ΓM and ΓK is a = (3.25 ± 0.05) Å. Within experimental error, the MoS_2 lattice parameter was found to remain constant in the temperature range between 90 and 522 K [1], in good agreement with previously reported DFT based calculations [2].

In addition, by measuring specular interference between adjacent terraces, we were able to determine the step height at the surface (d = 12.10 Å), which means that mechanical exfoliation of our samples led mainly to formation of double layer steps.

References:

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[2] L. F. Huang, P. L. Gong and Z. Zeng Phys. Rev. B **90** 045409 (2014)