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Very High Frequency EPR Measurements on MoS_2 Bulk Crystals

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Introduction

The broad current interdisciplinary research effort on layered two-dimensional (2D) transition metal dichalcogenides (TMDs) such as MoS_2 and WS_2 is a hot topic in the community for next generation nano-electronic devices beyond CMOS.[1] Defects play a major role in these materials. Identifying them is the task of this work. This study aims to identify paramagnetic point defects at the atomic level in MoS_2 bulk crystals using very high frequency (120-500 GHz) Electron Paramagnetic Resonance (EPR) spectroscopy available at NHMFL, for the first time. Very high frequency EPR spectroscopy is highly sensitive technique to identify defects, which contain unpaired spins due to its enhanced sensitivity and resolution, compared to low frequency (~ 9 GHz) EPR.

Experimental

The heterodyne spectrometer at the EMR facility was used, based on the 12.5 T SC magnet. The specific frequencies were 120 and 240 GHz, the fields 4 - 9.5 T and temperatures 5 - 40 K.

Results and Discussion

Properties of TMDs such as MoS_2 have shown to be tunable depending on the type of defect present within the bulk sample when the exfoliation method is applied to make different devices. Most of the devices made from MoS_2 layers obtained from the exfoliation of MoS_2 bulk crystals. This work deals with the atomic level identification of different defect sites that are present within the same bulk sample, but in the different pieces of the same MoS2 crystals. We used very high EPR spectroscopy to identify these defect sites. Our comprehensive experimental findings show that some pieces of naturally occurring MoS_2 bulk crystals show Nb paramagnetic defects (see **Fig.1**). Interestingly, other pieces show Pb paramagnetic impurities and sulfur vacancies.[2,3] This study strongly suggests considering the nature of these defects when accounting for optoelectronic and chemical properties of 2D materials. Measurements were extended to MoS_2 nanocrystals also.

Conclusions

This work shows that different pieces from the same bulk MoS_2 crystals contain different paramagnetic defect sites that can completely alter the electrical properties of devices made from this material. As is the case from the Nb and Pb defects we observed, since Nb is known to act as an acceptor and Pb as a donor. These factors must be taken into consideration when constructing different devices with naturally grown MoS_2. This work is the first to demonstrate that Nb and Pb extrinsic defects present in geo-MoS_2 crystals.

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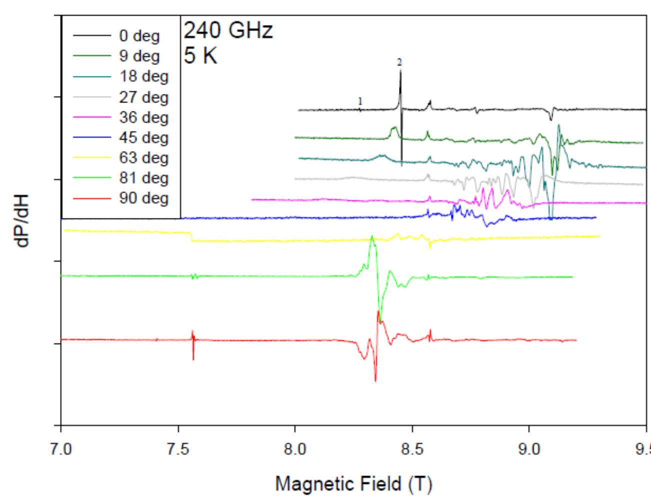

Fig.1 Angle dependence of EPR spectra collected on MoS_2 bulk crystal measured at 5 K, 240 GHz.