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Probing the interlayer coupling in two-dimensional layered 2H-MoS_2 and 2H-WS_2 by EXAFS and reverse Monte Carlo simulations

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Introduction

Two-dimensional (2D) layered materials, including transition metal dichalcogenides, have attracted considerable interest during the last decades due to their extraordinary electronic, optical, transport, and tribological properties. The structure of these materials (**Fig. 1**) is characterized by strong in-plane covalent chemical bonds and **weak van-der-Waals (vdW)** interactions between layers.

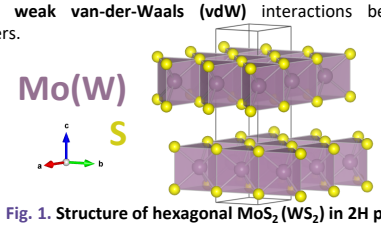

Fig. 1. Structure of hexagonal MoS_2 (WS_2) in 2H phase (space group 194, $P6_3/mmc$).

X-ray absorption spectroscopy (XAS) has been used in the past to probe the short-range order in 2D materials. However, the conventional approach to XAS data analysis, based on multi-shell modeling, cannot provide reliable information on the long-range (across the vdW spacing) interlayer interactions due to a strong correlation between model parameters for distant coordination shells. At the same time, the extraction of such information is possible using an advanced approach, since the range of atomic structure around the absorbing atoms probed by XAS extends up to 10-15 Å, being limited by the photoelectron mean-free path (**Fig. 2**).

In this study, we demonstrate the possibility to extract temperature dependence (10–300 K) of intralayer and interlayer interactions in 2D **2H-MoS_2** and **2H-WS_2** from the analysis of the Mo K-edge and W L_3-edge EXAFS spectra using the **reverse Monte Carlo (RMC)** simulations [1].

Conclusions

- **High-quality experimental data for 2H-MoS_2 and 2H-WS_2 were obtained during XAS measurements at PETRA III synchrotron P65 beamline.**
- **Good agreement between experimental and theoretically calculated EXAFS spectra was obtained during RMC simulations.**
- **The analysis performed up to the 10th coordination shell allowed evaluation of EXAFS sensitivity to interactions between atoms located in different layers.**
- **Mean-square relative displacement (MSRD) factors for atom pairs located in the same or neighbouring layers differ significantly indicating a drastic reduction of correlation between distant atoms.**

References

[1] J. Timoshenko, A. Kuzmin, J. Purans, J. Phys.: Condens. Matter 26, 055401 (2014).

EXAFS data

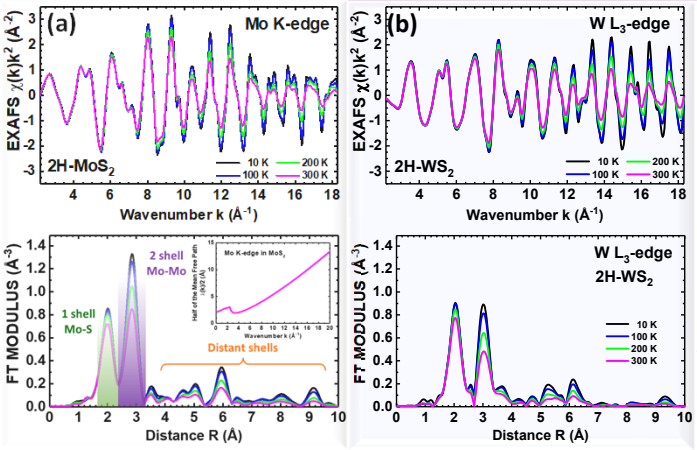

Fig. 2. Temperature-dependent experimental Mo K-edge and W L_3-edge EXAFS spectra and corresponding Fourier transforms (FTs) of 2H-MoS_2 (a) and 2H-WS_2 (b). Calculated half of the effective mean-free path of the photoelectron in 2H-MoS_2 is shown in the inset. Data were obtained at PETRA III synchrotron P65 beamline (c).

Results of reverse Monte Carlo calculations

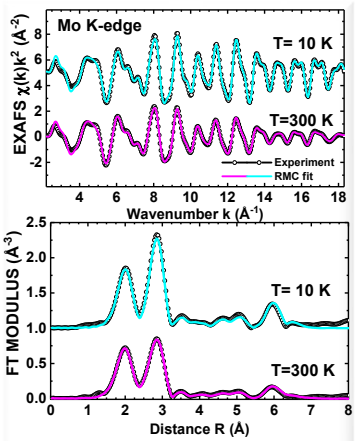

Fig. 3. Comparison of the experimental and with RMC method simulated EXAFS spectra and corresponding FTs.

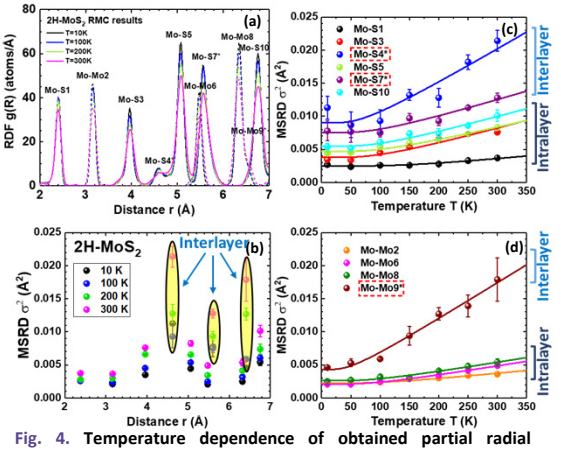

Fig. 4. Temperature dependence of obtained partial radial distribution functions (RDFs) around absorbing Mo atoms in 2H-MoS_2 (a). Calculated MSRD factors as a function of radial distance (b) and temperature (c,d). Solid lines are fits by the correlated Einstein model.

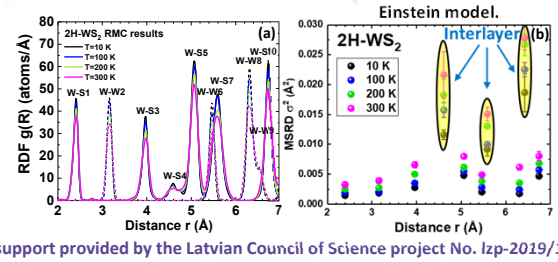

Fig. 5. Temperature dependence of partial RDFs around absorbing W atoms in 2H-WS_2 (a). Calculated MSRD factors as a function of radial distance (b).

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