Localized electronic state of Mo_{1-x}Re_xS₂ monolayer

studied by STM/STS

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Recently, atomically thin transition metal dichalcogenides (TMDs) has been attracted much attentions due to their desirable semiconducting properties such as high optical absorption coefficient, efficient photoluminescence. Engineering such electronic/optical properties has been realized by forming alloy and heterostructure combining various transition metals (Mo, W, Re) and chalcogen atoms (S, Se, Te). In addition, phase engineering has recently been proposed for further control of their property since TMDs has various polymorphs (2H, 1T, 1T'). For understanding the basic stage of phase engineering, it is necessary to study how alloying between different polytype TMDs affects atomic and electronics structure.

In this study, we performed STM/STS measurements on $Mo_{1-x}Re_xS_2$ (Re=7%) alloy monolayer. Because of a phase segregation during CVD growth, $Mo_{1-x}Re_xS_2$ partially forms 2H phase in Mo-rich regions and 1T' phase in Re-rich regions. Fig.1 shows STM image of Mo-rich area where 2H phase was formed ($V_s = -1.5V$). Re atoms are imaged as bright protrusions in filled state image due to their localized state. Fig.2 shows dI/dV spectrum obtained on the areas indicated by arrows in Fig.1. Two unique peaks within the gap of host MoS_2 were observed on Re atoms. As shown in fig.2, peak strength and position were strongly influenced by the number of adjacent Re atoms and prominent deep state was observed especially on Re trimmer. To clarify the origin of these states, we have carried out DFT calculation. And the results revealed that these states are caused by lattice distortion locally induced around Re atoms. Further details will be discussed in the presentation





Figure 1. STM image of Mo_{1-x}Re_xS₂ monolayer

Figure 2. dI/dV spectrum obtained on the area indicated by each arrows in fig.1