Localized electronic state of Re dopant in monolayer MoS_2 studied by STM/STS

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According to Moore's law "The density of semiconductors doubles in 1.5 years", LSI made of Si have been integrated. However, miniaturization of semiconductor device is going to reach its limits. Against this backdrop, the expectation for layered materials such as graphene has been increased in developing high performance and small-sized semiconductor devices. Among others, 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. Towards these device applications, it is necessary to control the electrical characteristics of MoS_2 by doping. Although Re is expected to be n-type dopant, understanding of its electronic state has not yet advanced. In this study, we observed the atomic structure and electronic state of Re doped monolayer MoS_2 by STM and compare with the result of DFT calculation.

In this study, we performed STM/STS measurements on CVD grown MoS_2 (Re=7%) alloy monolayer. Fig. 1 shows an STM image of a single layer MoS_2 doped with Re atoms. The Re atom is observed brighter than MoS_2. Its shape represents the local electronic state of the Re atom and it can be classified into the three types shown in Fig. 2. Each type reflects the difference in the local structure of the dopant. From the STM image it can be determined that the A type accounts for 94% of the total, and from the comparison with the TEM measurement result of the previous study, it was thought that A has Mo substitution type structure. Fig. 3 shows the results of STS measured on Re atom and MoS_2. On the Re atom, both the valence electron edge and the conduction band edge changed in the direction of narrowing the apparent band gap and the effect became more prominent in the region where the Re atoms were adjacent, as compared with MoS_2. This result is due to the formation of a shallow gap level near the valence band edge in addition to the initially expected donor level of Re dopant. The results of the DFT calculation suggested that the shallow gap level is due to the lattice distortion around Re atoms.

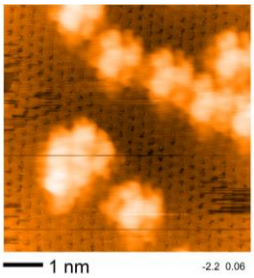

Figure 1. STM image of MoS2 monolayer (Vs=--2.2V)

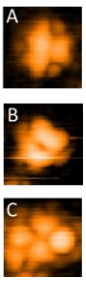

Figure 2. Classification of Re dopant by STM image

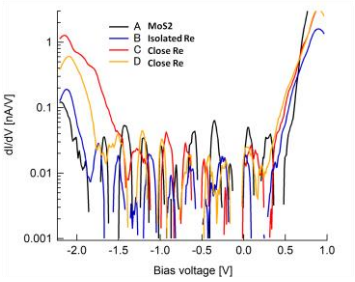

Figure 3. dI/dV spectrum measured on Re atoms and MoS2