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Ultrathin NiO films on Ag(001): defects and electronic structure

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We study the early stage of the NiO growth on Ag(001) by high resolution photoelectron spectroscopy. O 1s sprectra of NiO films on Ag(001) has the shoulder peak which has higher binding energy at 110K. It had been considered as the contamination or the physisorbed O_2. However, we can observe that the shoulder peak is larger after the temperature became higher. It means that it is related with Ni oxide phase, not just contamination. Now, we further identify the defect positions of NiO ultrathin films as the origins of such structures.

In addition, we investigate the valence band structuer to study metal-insulator transition; we built the films of various thickness. We found the transition in between 2.0ML and 2.5ML. This experiment suggests the Coulomb interaction energy U; by LDA + U calculation, the Coulomb interaction energy U smaller than the bulk NiO can explain we observed metal-insulator transition.