STEM Structural Study of MgO/NiO/YZO Polar Thin Films

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Polar oxide interfaces have recently attracted a lot of attention due to their unique non bulk electronic properties [1]. The existence of novel electronic properties at polar oxide interfaces, such as 2D electronic gas, is being considered to be result of the abrupt change of the electrostatic potential across the interface [2], or due to building up of electrostatic potential that is proportional to film thickness [3]. Among the various polar oxide systems, the most thoroughly studied are the perovskite type of polar oxides due to experimentally demonstrated existence of 2D electronic gas at STO/LSO type of the interfaces [1]. However, beside perovskite classical system, not much research has been done of systems such as spinel, wurtzite and rock salt polar oxide structures. Main obstacle in the experimental realization of number of polar oxide structures/interfaces is the inability to grow well defined structural polar oxide films due to high surface energy of polar oxides in general. Recently several successful studies have been reported on the growth and stability of polar MgO(111) thin films [4,5]. These findings open the possibility to create rock salt type of polar oxide interfaces which electronic properties are yet to be explored. The very first question that has to be answered is whether these types of interfaces are structurally abrupt and thermodynamically stable. In these letter we used MgO/NiO/YZO as a model rock salt polar oxide interface to study the chemical and structural abruptness of the interface and the structure of the films.

Film growth has been done by pulse laser deposition on Yttria stabilized zirconia oxide (YZO). After the growth the films were annealed at 1000 C in order to achieve film structural homogeneity. Films and interface atomic structures were studied bt TEM/STEM methods using double aberration corrected JEOL 2200FS microscope Also density functional theory was used to analyze stability of several model interfaces including abrupt and mixed interfaces.

Fig. 1 shows low magnification cross sectional HAADF image of the MgO/NiO/YZO films. Both NiO(111) and MgO(111) films were grown epitaxially to each other and to the YZO substrate. Both films have uniform thickness and their roughness is very well controlled, result also confirmed by RHEED. Interface between NiO(111)/YZO(111) is shown in Fig.2. Due to the very large mismatch between NiO and YZO (~20%) an interfacial network of misfit dislocation is formed at the NiO/YZO interface that very efficiently release the strain in the NiO film. It can be seen that dislocation are periodically formed on every 4 and 5 atomic plane at the interface. Assigning the high Z contrast to Y/Zr and lighter to Ni atomic columns, interface models can be deduced from the inset of Fig.2. In contrast to NiO/YZO the MgO/NiO interface is not as sharp. Ongoing work is carried on in order to establish whether this interface is inherently stable and under what conditions. The DFT modeling indicates possible mixing as a function of the MgO-NiO interface crystallographic orientation.

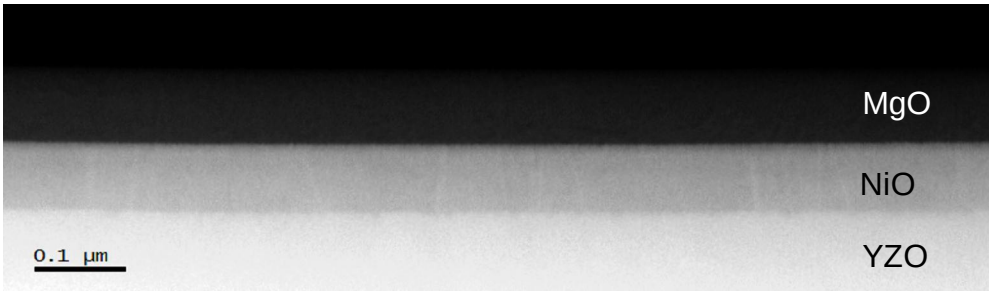

FIG.1. Low magnification HAADF image from MgO/NiO/YZO multilayer film.

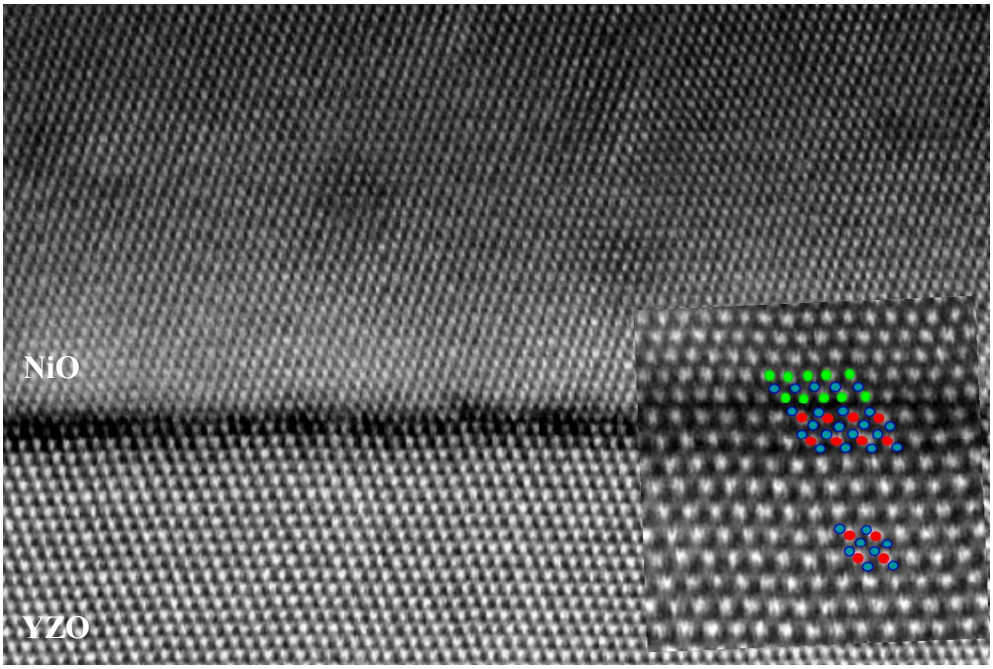

FIG.2 a) HAADF from the NiO(111)/YZO(111). b) HAADF from the near interface region from NiO/YZO showing the abruptness of the interface and its atomic structure. Filled circles represent atomic column of O (blue), Y/Zr (red), and Ni (green).

References

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