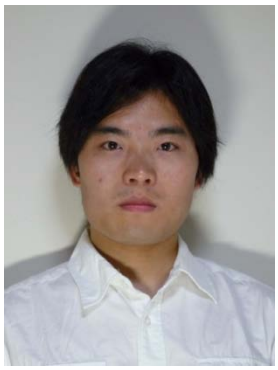
中心系列讲座

[illegible]



[illegible]

WPI Research Center
Advanced Institute for Materials Research
Tohoku University

[illegible]

Abstract

Local atomic structure, chemistry and bonding at interfaces or grain boundaries can often radically alter properties of materials. However, to catch such an impact on an atomistic level remains extremely challenging. Although the direct imaging using scanning transmission electron microscopy (STEM), the highest resolution so far , makes the atomic-scale characterization a reality, it is still not always straightforward to interpret the observed images especially in the case of interfaces, for which their own complications might cause incomplete imaging. Here we combine the advanced STEM image with additional first-principles calculations to address structure of a few technologically important interfacial systems and relate it to property on atomic level.

The interfacial systems involve the functional SiC/Ti3SiC2 interface, A-site excess, nonstoichiometric oxides, La0.5Srn+1-0.5TinO3n+1, and grain boundaries in MgO. The SiC/Ti3SiC2 interface is important because it can facilitate the formation of Ohmic contact, which has been a long-standing issue limiting the device processing in SiC technology. The formation of the Ohmic contact is attributed to an epitaxial, coherent and atomically ordered interface, which can trap even atomic monolayer of carbon. The La0.5Srn+1-0.5TinO3n+1 oxides present an unexpected insulator-to-metal transition that is driven by an intrinsically insulating unit cell . The transition is accompanied by electron localization due to the strain-induced lattice distortion, and is unusual as the majority of electrons in the conducting phase are confined forming a two dimensional electron gas. As for the MgO grain boundary, an ordered defect superstructure is spontaneously clustered, affecting fundamentally the intrinsic electronic properties of MgO.

About the Speaker

Dr. Wang received his Bachelor degree from Anhui University of Technology in 2001 and his PhD from University of Tokyo in 2007. After working as a postdoctoral fellow in Tohoku University, he works as an assistant professor in NANO Interface Technology Group World Premier International Research Center, Advanced Institute for Materials Research, Tohoku University . His current research interests are (1) Density-functional-theory (DFT) calculations (+U) on functional materials;(2) Fabricate layered oxides via pulsed laser deposition (PLD), and investigate the metal-insulator transition