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**Direct Imaging and First Principles Studies of $Si_3N_4/SiO_2$ Interface**[1] WERONIKA WALKOSZ, ROBERT KLIE, SERDAR OGUT, University of Illinois at Chicago, BILIJANA MIKIJELJ, Ceradyne Inc., STEPHEN PENNYCOOK, JUAN C. IDROBO, Oak Ridge National Laboratory — It is well known that the composition of the integranular films (IGFs) in sintered polycrystalline silicon nitride ($Si_3N_4$) ceramics controls many of their physical and mechanical properties. A considerable effort has been made to characterize these films on the atomic scale using both experimental and theoretical methods. In this talk, we present results from a combined atomic-resolution Z-contrast and annular bright field imaging, electron energy-loss spectroscopy, as well as ab initio studies of the interface between $\beta$-$Si_3N_4$(10-10) and $SiO_2$ intergranular film. Our results show that O replaces N at the interface between the two materials in agreement with our theoretical calculations and that N is present in the $SiO_2$ IGF. Moreover, they indicate the presence of atomic columns completing $Si_3N_4$ open rings, which have not been observed experimentally at the recently imaged $Si_3N_4$/rare-earth oxides interfaces, but have been predicted theoretically on bare $Si_3N_4$ surfaces. The structural and electronic variations at the $Si_3N_4/SiO_2$ interface will be discussed in detail, focusing in particular on bonding characteristics.

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