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Characterization of Silicon Nitride/Lanthanide-Oxide Interfaces at the Atomic Scale by Scanning Transmission Electron Microscopy and Density Functional Theory J. C. IDROBO, University of Illinois at Chicago, A. ZIEGLER, UC Davis, M. CINIBULK, Air Force Research Laboratory, C. KISIELOWSKI, NCEM Lawrence Berkeley National Laboratory, R. RITCHIE, UC Berkeley and NCEM Lawrence Berkeley National Laboratory, N. BROWNING, UC Davis and NCEM Lawrence Berkeley National Laboratory, S. OGUT, University of Illinois at Chicago — $\beta-Si_3N_4$ ceramics are good candidates for heat- intensive structure applications. However, the wide use of the material is limited by its brittleness. This can be compensated by the addition of secondary rare-earth oxide phases into the Si_3N_4 matrix. We investigate the bonding of different rare-earth atoms to the interface between the Si_3N_4 matrix grains and the intergranular phase doped with La, Sm, Er, Yb, and Lu. Using atomic resolution Z-contrast imaging and EELS in the STEM and density functional theory, we find, for the first time, how each rare-earth element attaches to the interface differently depending on atomic size, electronic configuration, and the presence of oxygen along the interface. Atomic resolution EELS taken at the interface suggest that the electronic structure of the rare-earth dopants plays a secondary effect on the positioning of the atoms at the interface. The Si L_{23} edge signal from the termination position has Si−O-like features indicating that the open hexagonal Si_3N_4 rings are oxygen terminated. This result is also confirmed by DFT calculations.

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