Identification and lattice location of oxygen impurities in $\alpha$-Si$_3$N$_4$

MARK P. OXLEY, JUAN C. IDROBO, Vanderbilt U., W. WALKOSZ, ROBERT F. KLIE, SERDAR OGUT, University of Illinois at Chicago, BILJANA MIKIJELJ, Ceradyne Inc., STEPHEN J. PENNYCOOK, ORNL, SOKRATES T. PANTTELIDES, Vanderbilt U. — For over 40 years impurities have been believed to stabilize the ceramic $\alpha$-Si$_3$N$_4$, but there is no direct evidence for their identity or lattice location. In bulk materials electron microscopy can generally image heavy impurities. Here we report direct imaging of N columns in $\alpha$-Si$_3$N$_4$ that suggests the presence of excess light elements in specific N columns. First-principles calculations rule out Si or N interstitials and suggest O impurities, which are then confirmed by atomically-resolved electron energy-loss spectroscopy. The result provides a possible explanation for the stability of $\alpha$-Si$_3$N$_4$ with implications for the design of next-generation structural ceramics.

Research supported by NSF (DMR-0605964 & DMR-0513048), the Office of Basic Energy Sciences, Div. of Mat. Sciences and Eng., the SHaRE User Facility, US. DOE, and by the McMinn Endowment at Vanderbilt University. Computations were supported by NERSC.