Atomic Scale Characterization and First-Principles Studies of Si?N? Interfaces (Springer Theses)

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This thesis presents results from a combined atomic-resolution Z-contrast and annular bright-field imaging and electron energy loss spectroscopy in the Scanning Transmission Electron Microscopy, as well as first principles studies of the interfaces between crystalline β–Si_3N_4 and amorphous (i) CeO2-x as well as (ii) SiO2 intergranular film (IGF). These interfaces are of a great fundamental and technological interest because they play an important role in the microstructural evolution and mechanical properties of Si3N4 ceramics used in many high temperature and pressure applications. The main contribution of this work is its detailed description of the bonding characteristics of *light* atoms, in particular oxygen and nitrogen, at these interfaces, which has not been achieved before. The atomic-scale information on the arrangement of both light and heavy atoms is critical for realistic modeling of interface properties, such as interface strength and ion transport, and will facilitate increased control over the performance of ceramic and semiconductor materials for a wide-range of applications.

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