

Hanau, FRG for a stimulating and fruitful cooperation. The financial support from the Swedish Natural Science Council (NFR) and from the Swedish Board for Technical Development (STU) is also gratefully acknowledged.

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Summary Abstract: Effect of oxygen incorporation in AlN thin films

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(Received 19 November 1987; accepted 21 December 1987)

The effects of oxygen on the physical properties of AlN is of increasing technological importance. We have studied AlN thin films with a range of oxygen doping from oxygen-free to AlN_xO_y and γ -Al₂O₃. Core and valence-band photoelectron spectroscopy, UV optical transmission, and ellipsometry have been utilized to investigate the effects of oxygen incorporation. The absorption edge (AE) and the valence-band maximum (VBM) stay constant for oxygen-free AlN and low oxygen doping, indicating that the composition of solid solution does not affect the optical properties or the electronic structure. At higher levels, both AE and VBM shift toward higher energies upon forming γ -Al₂O₃, thus increasing the band gap.

Recent developments in AlN synthesis have raised the question as to a role of additives in the ceramic processing of AlN. The incorporation of oxygen impurities in AlN has received considerable attention since lattice oxygens have been shown to degrade the thermal conductivity of AlN. The identification of oxynitride or oxide phase formation is of fundamental interest for these questions. We have chosen polycrystalline thin-film AlN as a model system to study the effect of oxygen doping on the properties of AlN. In addition AlN and Al₂O₃ are the end members of a compositional family, encompassing aluminum oxynitride. We have combined our knowledge with measurements of the optical and valence-band properties to determine the electronic structure changes associated with oxygen incorporation in AlN.

Polycrystalline AlN thin films were grown by reactive sputter deposition of an Al target in a nitrogen plasma. Oxygen doping during synthesis was made by presetting the oxygen pressure in the sputtering chamber prior to introducing the sputtering gas. The background pressure of the system was low 10⁻⁷ Torr. Other sputtering conditions were rf power of 500 W, total pressure of 5 μ , and sputtering gas mixture (Ne + 35% N₂). An aluminum oxide thin film was

also made for comparison from an Al₂O₃ target in (Ar + O₂) sputtering gas mixture. The thin films were 0.1–1 μ thick on Si, Suprasil I (SiO₂), and sapphire substrates.

We have utilized a battery of techniques to characterize the thin films. Thin-film structure and orientation were determined by conventional x-ray diffraction techniques. High-resolution x-ray diffraction was also performed using the synchrotron light source at Brookhaven National Laboratory. The average strain along the *c* axis was calculated from a relationship $\epsilon = (c - c_0)/c_0$, where *c*₀ is the lattice constant of unstrained AlN, 4.9752 Å. Refractive indices were measured using ellipsometry at 642.8- and 441.6-nm lights. The stoichiometry of the thin film was determined by Auger electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS), while that of the optical band gap was determined by vacuum ultraviolet (VUV) absorption measurements.

The properties of the thin films are summarized in Table I. The oxygen concentration in the film is seen to change dramatically with increasing gas phase oxygen concentration. These changes in the rate of oxygen incorporation with increasing gas phase oxygen activity are associated with the formation of new phases. The transition from AlN to Al₂O₃ through an AlON phase is recognized clearly by the change in the refractive index and the optical band gap. We found that the index of refraction was insensitive to the oxygen doping up to 8% content in the film, indicating the film is still bulk AlN. Beyond this value, the refractive index drops sharply. The measurement of the absorption edge and band gap of the films shows a similar trend. For low oxygen contents (< 8%), the band gap was 5.8 eV and a similar absorption edge was observed; while at 33% oxygen content, the band gap slightly increased to 6.2 eV, but there is a pronounced change in the absorption edge. At 63% oxygen content, the band gap has moved dramatically to higher energy