602c Impurity Incoporation during the Sublimation Growth of Aluminum Nitride Crystals

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Single crystal aluminum nitride is superior to sapphire and silicon carbide as a substrate for AlxGa1-xN based electronic and optoelectronic devices, because of its similar lattice constants, good thermal stability, high electrical resistivity and high thermal conductivity. Since it has the same wurtzite crystal structure as AlxGa1-xN, AlN substrates are not limited to (0001) orientations; it can be employed for epitaxy on nonpolar crystal planes as well. Furthermore, AlN is not a potential source of impurities during epitaxy, since it shares the same elements as AlxGa1-xN. Here, the most probable impurity vapor phase species were predicted by Gibbs free energy minimization. Furthermore, the distribution of impurities between the source and the crystals was experimentally determined. Bulk AlN crystals are produced at temperatures greater than 2000 °C, thus impurities can be introduced into the growth environment from reactions between aluminum vapor, nitrogen, the heating element, crucibles, and retorts, as well as from the AlN source. Oxygen and carbon are the impurities present in the highest concentration in both the source and the crystals. Due to aluminum's strong affinity for oxygen, dialuminum monoxide (Al2O) is strongly favored over all other possible oxygen containing compounds including CO and NO. Dialuminum monoxide is highly volatile, thus partial sublimation of the source material reduces its oxygen concentration by almost two orders of magnitude. Gas-phase carbon species (cyanogen (CN) and dicyanogen (C2N2)) forms from its reaction with nitrogen; this reaction is particularly important if the furnace contains any graphite. Aluminum nitride crystals grown in tungsten crucibles in a tungsten furnace (ie carbon-free) typically have oxygen and carbon concentrations of 0.03 wt% and 0.006 wt%, approximately 100 and 10 times lower than the original source materials. Analysis of the volatility of other common elements such as tungsten and silicon will also be discussed.