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Synthesis and Characterization of $\text{Zr}_{1-x}\text{Si}_x\text{N}$ Thin Film Materials

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— A series of zirconium silicon nitride ($\text{Zr}_{1-x}\text{Si}_x\text{N}$) thin films were grown on r-plane sapphire substrates using rf magnetron co-sputtering of Zr and Si targets in a N_2/Ar plasma. The films were grown at 200°C and also post-deposition annealed at 1000°C for 2 hours in vacuum. Pure face-centered cubic ZrN grows with high quality (100) epitaxy on r-plane sapphire as demonstrated by X-ray diffraction (XRD) pole figure analysis. Small amounts of Si (up to 6%) added to the ZrN lattice cause the $\text{Zr}_{1-x}\text{Si}_x\text{N}$ films to become polycrystalline, whereas higher amounts of Si (above $\sim 15\%$) cause the films to become amorphous. X-ray photoelectron spectroscopy (XPS) measurements were used to determine film stoichiometry and provide information about chemical bonding. The Auger parameters for N, Zr, and Si decrease as a function of Si content suggesting the formation of a more polarized bond. Optical microcopy and atomic force microscopy revealed smooth films except for Si concentrations corresponding to where the film transforms from polycrystalline to amorphous structure. At this transition, evidence is found for film delamination and hillock formation. UV-visible optical absorption spectroscopy showed a direct correlation between the location of the absorption edge and magnitude of the optical band gap and the Zr/Si composition ratio.

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