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Tailoring the Optical and Structural Properties of Si-Doped HfO₂ Films by Hydrogen-Assisted Magnetron Sputtering and Post-Annealing treatment

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The optical and structural properties of Si-doped HfO $_2$ thin films were systematically investigated as a function of deposition conditions and post-deposition annealing. The films were deposited by RF magnetron sputtering of a composite Si:HfO $_2$ target in pure Ar or Ar–H $_2$ plasma. Structural, optical, and luminescent characteristics were examined using spectroscopic ellipsometry, photoluminescence, Fourier transform infrared spectroscopy, and transmission electron microscopy. The Si content in the films was controlled either by varying the Si:HfO $_2$ target composition or by adjusting the hydrogen flow during sputtering. The former approach increased the refractive index up to 2.42 (at 1.95 eV), while hydrogen incorporation further enhanced it to about 2.7, compared with 1.98–2.00 for undoped HfO $_2$. Annealing in nitrogen at 400–900 °C preserved the amorphous and chemically homogeneous structure, demonstrating high thermal stability and suitability for optical device integration. At higher annealing temperatures (up to 1100 °C), phase separation occurred, leading to the formation of distinct HfO $_2$ and SiO $_2$ phases. Alternating deposition in Ar and Ar–H $_2$ plasmas enabled the fabrication of multilayered Si-doped structures from a single composite target, allowing controlled variation of the sublayer composition. For films with elevated Si content, a narrow processing window was identified that favored the formation of highly Si-rich phases. These results revealed the promising properties of Si-doped HfO $_2$ materials for tunable optical applications.

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