Optical and structural properties of group-IV oxides produced by rapid thermal oxidation

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There is great interest in germanium and germanium-tin alloys as optical sensors, especially short-wave infrared detectors, but little is known about thermal oxidation of thin Ge-Sn alloy layers on a bulk semiconductor substrate. We report a comparative study of the rapid thermal oxidation of bulk Ge, thick relaxed epitaxial Ge on Si, and Ge-Sn alloys on Si produced by chemical vapor deposition. Layer thickness, roughness, composition and strain, optical constants, and infrared-active molecular vibrations were characterized using spectroscopic ellipsometry, high-resolution x-ray diffraction, atomic force microscopy, and Fourier-transform infrared spectroscopy.

Before oxidation, the surfaces were ultrasonically cleaned in deionized water at room temperature and dried with nitrogen to achieve a low native oxide layer with less than 1 nm thickness. The ellipsometric angles ψ and Δ were acquired on a J.A. Woollam vertical angle spectroscopic ellipsometer (VASE) from 0.5 to 6.5 eV and on a J.A. Woollam Fourier-transform infrared spectroscopic ellipsometer (FTIR-VASE) from 0.03 to 0.6 eV at incidence angles ranging from 60-80°. The ellipsometric angles were then modeled with a three-layer model: Si substrate, pure Ge (or Ge-Sn) layer, and GeO_2, to obtain initial conditions. The initial strain was determined using high-resolution x-ray diffraction (HRXRD), including symmetric (004) and asymmetric (224) reciprocal space maps and rocking curves.

The samples were then rapidly thermally annealed in pure oxygen at temperatures ranging from 525-575°C in 40 psi pressure for up to 2 hours to create a range of thermal oxide layers on different types of surfaces. After oxidation, HRXRD and ellipsometric angles are measured again and compared to pre-oxidation results.

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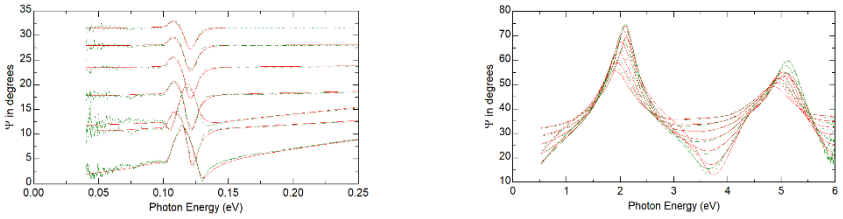

Figure 1. Ellipsometric angle ψ of the dielectric function for thermally annealed bulk germanium in the IR range (left) and UV range (right).