Optical and X-Ray Characterization of Pseudomorphic $Si_{1-x}Ge_x$/Si

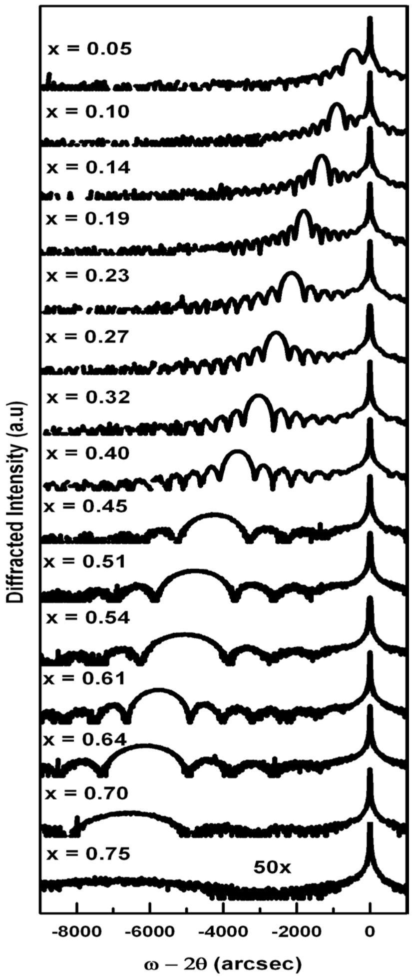
A.C. Diebold, G. Muthinti, M. Medikonda, and T.N. Adam
College of Nanoscale Science and Engineering
257 Fuller Road, Albany, NY USA
518-956-7363 adiebold@albany.edu

A. Reznicek
IBM Research at Albany Nanotech,
257 Fuller Road, Albany, NY USA

Here we review the X-Ray Diffraction and optical characterization of Pseudomorphic $Si_{1-x}Ge_x$/Si and $Ge_{1-x}Sn_x$/Ge epilayers. Truly pseudomorphic epilayers have in-plane lattice constants that match that of the substrate wafer. When the lattice mismatch between epilayer and substrate is large, the biaxial stress is significant. It is difficult to grow truly epitaxial layers, and therefore we discuss the X-Ray measurements that prove the pseudorphic nature of the films. Stress is known to alter the optical properties (dielectric function / complex refractive index) of semiconductors. The goal of this work is to develop and understanding of the impact of stress on the complex dielectric function using spectroscopic ellipsometry.

The first step in this characterization is to use high resolution X-Ray diffraction to prove the pseudomorphic nature of the epi layers. Triple axis (004) ω - 2θ rocking curves were used to determine the lattice constant and thickness of the epi layers. The symmetric 004 reflection measures the lattice spacing perpendicular to the sample surface. The peak position of the SiGe (004) diffraction determines the lattice constant and because these films are pseudomorphic it also allows calculation of Ge content. The low defect density and highly ordered nature of the epi layer allows thickness determination from the period of the interference fringes. The (004) ω - 2θ rocking curves for $Si_{1-x}Ge_x$/Si are shown in Figure 1. We further characterized the layers using reciprocal space maps (RSM). Reciprocal space maps confirmed zero percent relaxation in all the wafers and showed that they are fully strained. The relaxation scan analyzes additional asymmetric reflection information from 224 planes along with the symmetric 004 scan and checks if the layer's parallel lattice parameter is identical to that of the Si substrate. If the layer is relaxed, the parallel lattice parameter will not be matched, but the substrate crystal orientation will match the layer crystal orientation. The (004) and (224) RSMs for $Si_{1-x}Ge_x$/Si are shown in Figure 2.

The dielectric function (complex refractive index) is altered in the pseudomorphic $Si_{1-x}Ge_x$/Si epilayers. Stress is known to shift the energies of direct gap critical point transitions that dominate the dielectric function of semiconductors. The biaxial stress in pseudomorphic films grown on silicon wafers can be as high as that used during stress studies of the optical properties of bulk semiconductors. The amount of stress in un-relaxed, pseudomorphic films of $Si_{1-x}Ge_x$ on Si (100) reaches 1 GPa for alloys with 20% Ge and is more than 3 GPa for films with > 50% Ge. The bi-axial stress in sSOI is typically ~1 GPa. An elastic theory approach for the effect of strain on the k*p determined band structure and optical transition energy is well known. Both low shear stress and high shear stress approximations can apply to the shift in transition energy depending on the magnitude of the spin orbit splitting energy vs the magnitude of the shear stress. Here we discuss results from our recent study of pseudomorphic films of $Si_{1-x}Ge_x$ on Si (100) from x= 0.05 to 0.75 which covers both low and high shear regimes. The difference in the dielectric function between strained and unstrained $Si_{1-x}Ge_x$ on Si (100) is shown in Figure 3.



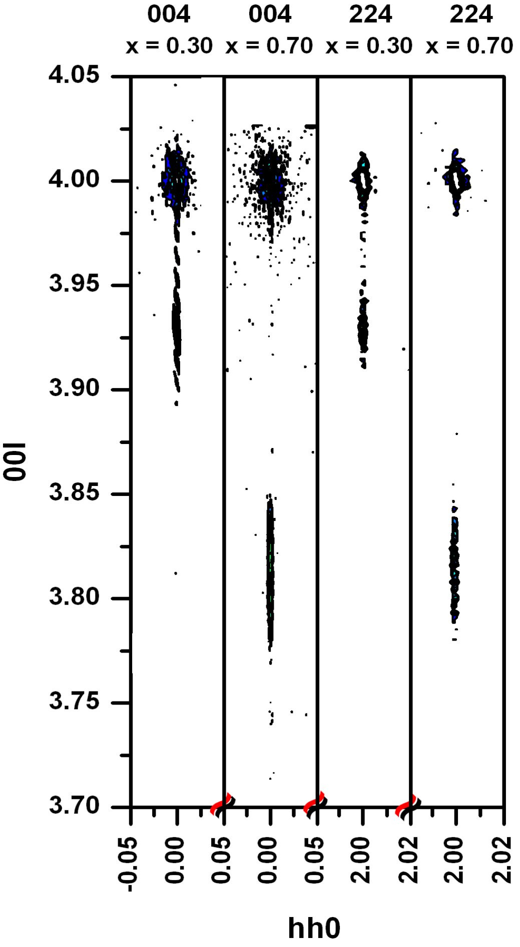


Fig. 1 Symmetric 004 rocking curves for selected Ge concentrations from the Si$_{1-x}$Ge$_x$ alloy films from x= 0.05 to x= 0.75.

Fig. 2 004 and 224 Reciprocal Space Maps showing the pseudomorphic nature of Si$_{1-x}$Ge$_x$ (x=0.3 and x=0.7) layer on Si Substrate. The 004 RSMs characterize the Si$_{1-x}$Ge$_x$ 004 lattice plane spacing for planes that are parallel to the Si 004 lattice planes while the 224 RSM characterizes quality of the lattice both parallel and perpendicular to the Si lattice.

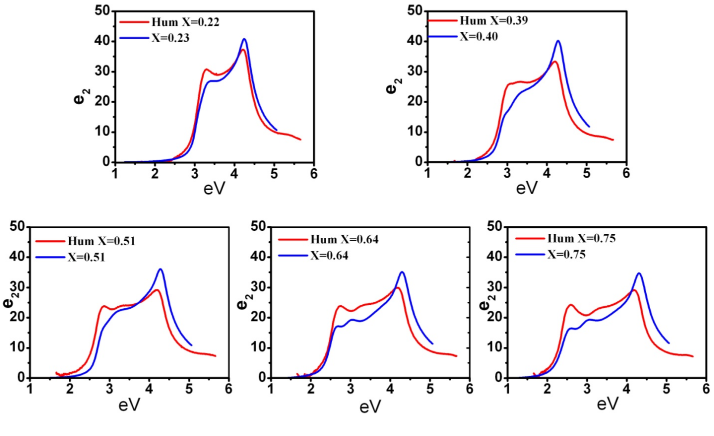


Figure 3: Comparison of the dielectric function of pseudomorphic Si$_{1-x}$Ge$_x$ alloys films with strain free Si$_{1-x}$Ge$_x$ alloys. The effect of strain on the line shape of the E$_1$ critical point is evident as the concentration of Ge increases. Hum refers to Humlicek's data for un-strained Si$_{1-x}$Ge$_x$.