Dielectric response of thick low dislocation-density Ge epilayers grown on (001) Si

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Spectroscopic ellipsometry was used to measure the dielectric functions of epitaxial and bulk Ge at photon energies from 1.5 to 5.2 eV. The epitaxial Ge was grown at 400 °C by molecular beam epitaxy on ~001! Si substrates. The optical response and the interband critical-point parameters of

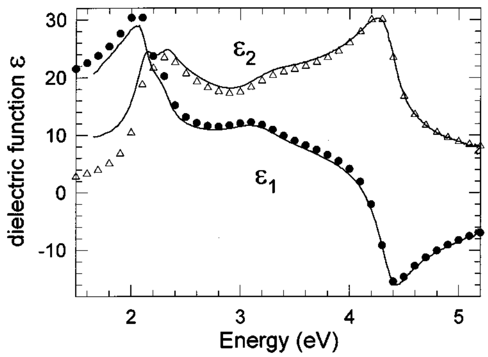

FIG. 1. Lines: Real (e_1) and imaginary (e_2) part of the dielectric function of SGC99 ~0.75 *m*m Ge on Si!, corrected for a 10 Å native oxide layer. The data of Ref. 13 for bulk Ge ^111& are shown for comparison (d),(n).

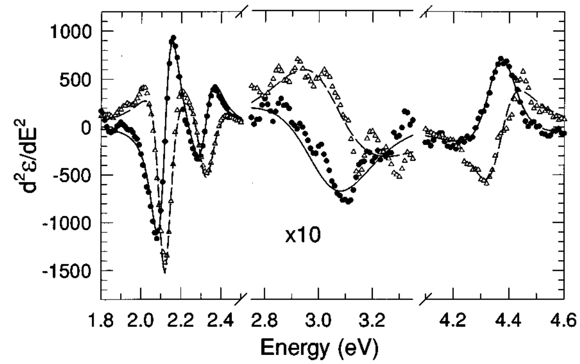

FIG. 2. Numerically calculated second derivatives of e_1 (d) and e_2 (n) for Ge on Si. The lines give the best fit to Eq. ~1! with the parameters in Table I. The E_0^8 region ~2.75–3.35 eV! was multiplied by 10 to make it visible on this scale.

Ge on Si grown at 400 °C, the RHEED pattern at the completion of growth was similar in features and intensity to that of commercially available Ge substrates. The RHEED suggested that island formation was partially suppressed at low growth temperatures, and that as growth proceeds islands may coalesce to form single crystal Ge with few defects. We speculate that the low growth rates employed here encourage the formation of reduced defect single crystal Ge over multicrystalline Ge, but further study will be necessary to confirm this.

To find the surface dislocation densities, we used an iodine etch[2] HF:HNO_3:CH_3COOH:I ~20 ml:40 ml:44 ml:120 mg! for 1 s to measure the etch pit density ~EPD! of the Ge layers. For SGC99, it appeared constant and uniform across the entire area and was consistent between samples and etch times. The average EPD was 4×10^4 cm^{-2}, a factor of five lower than the results of Malta *et al.*[2] The EPDs of thinner layers ($<$0.3 *m*m! and those of samples grown at higher temperatures ($>$500 °C! could not be determined, since the EPD was not uniform or the complete Ge layer was removed by the etch. The EPD of bulk Ge was less than 10^4 cm^{-2}, consistent with data supplied by Eagle Picher. The pit shapes for SGC99 and bulk Ge differed. For the bulk Ge, most pits were circular, about 1 *m*m in diameter. For SGC99, the pits were squares, approximately $1-3$ *m*m on each side.

After growth, the dielectric functions ~DFs! e in the 1.5 to 5.5 eV photon-energy range were measured *ex situ* with a spectroscopic ellipsometer.[13] The spectra were corrected for a native oxide layer. The thickness of the oxide was determined by matching e_2 at its peak near 4.2 eV with the data of Ref. 13. The lines in Fig. 1 show the real (e_1) and imaginary (e_2) parts of e for sample SGC99, assuming an oxide thickness of 10 Å. Other Ge epilayers grown on Si at the same temperature ~not shown in the figure! had similar e. For comparison, we also measured e for a commercial bulk Ge ^001& sample ~Eagle Picher!. The DF of SGC99 and that of the bulk sample were indistinguishable, except below 1.8 eV, where the accuracy of our instrument decreases. In Fig. 1 we also show the data of Ref. 13 ~d!, ~n! for bulk ^111& Ge. The agreement is good, except for e_2 in the range below 2 eV. ~Similar discrepancies were found in Ref. 16.! The DF of SGC99 resembles that of bulk Ge much more than that of thin Ge films enclosed between Si barriers.[14,15]

The spectra show a double-peak structure above 2 eV (E_1, E_1+D_1), a shoulder near 3 eV (E_0^8), and a third peak near 4.2 eV (E_2). These peaks are interband critical points ~CPs! arising from direct band-to-band transitions at various regions in the Brillouin zone.[17] For a further analysis of these CPs, we calculate numerically the second derivative of e with respect to photon energy ~shown by the symbols in Fig. 2! and perform a line shape analysis. Following Viña *et al.*,[17] we describe the CPs using a mixture of a 2D minimum and a saddle point represented by

$$e\sim v!=C-A\ \ln\sim\backslash v-E_g-iG!\exp\sim i f!, \qquad \text{~1!}$$

where $\backslash v$ is the photon energy, E_g the energy of the CP, G its broadening, A its amplitude ~oscillator strength!, and f the phase angle describing the amount of mixing. The parameters obtained from the line shape analysis are given in Table I in comparison with parameters of bulk samples from Viña and co-workers.[17] First, we note that our bulk parameters are, within the error bars, identical to those of Ref. 17 with one exception: Viña and co-workers used a fixed spin-orbit splitting $D_1=187$ meV determined from low-temperature measurements. In our analysis, we treated D_1 as

TABLE I. Critical point ~CP! parameters for bulk Ge and Ge on Si: amplitude ~A!, energy ~E!, broadening (G), and excitonic phase (F) @see Eq. ~1!#.

	A ~1!	*E* ~eV!	G ~eV!	F ~deg!
		Bulk Ge ~this work!		
E_1	5.5~3!	2.114~2!	0.058~2!	86~4!
E_1+D_1	4.1~6!	2.314~2!	0.076~6!	same
E_0^8	3.2~6!	3.05~2!	0.20~2!	−29~12!
E_2	8~1!	4.37~1!	0.107~1!	−193~11!
		Bulk Ge ~from Ref. 17!		
E_1		2.111~3!	0.06~1!	71~4!
E_1+D_1		2.298~3!	0.07~2!	same
E_0^8		3.11		
E_2		4.368~4!	0.109~9!	
		Ge on Si ~SGC99, this work!		
E_1	6.2~4!	2.116~2!	0.063~2!	84~4!
E_1+D_1	3.7~7!	2.322~2!	0.076~6!	same
E_0^8	3.3~5!	3.05~2!	0.21~2!	−29~9!
E_2	8~1!	4.37~1!	0.109~6!	−196~6!

a free parameter ~since it is a measure for the strain in the sample! and found $D_1 = 200$ meV for bulk Ge.

The CP parameters for sample SGC99 are similar to those of bulk Ge. Most importantly, the broadenings, related to defects, are essentially the same. Therefore, the scattering of electrons and holes in SGC99 was mostly due to intrinsic mechanisms such as electron-phonon interactions, not to sample imperfections such as dislocations, grain boundaries, impurities, etc. The spin-orbit splitting parameter for SGC99 was $D_1 = 206$ meV, about 3% larger than in bulk Ge. Using the small-shear approximation described in Ref. 11, we found upper bounds for the hydrostatic and ~001! shear strains (e_H and e_S) in SGC99. Since E_1 is the same for bulk Ge and SGC99, we conclude that the hydrostatic and ~001! shear shifts for E_1 (DE_H and DE_S) are approximately equal. Since ~the apparent splitting! D_1 changes by no more than 6 meV, DE_H and DE_S are about 3 meV each. We conclude that $|e_H| < 0.03\%$ and $|e_S| < 0.1\%$. Since $DE_H \} e_H$, whereas $DE_S \} e_S^2$ our estimate for e_S is less stringent than that for e_H. Using x-ray diffraction, the in-plane strain perpendicular to the growth axis ($e_{\cdot} = e_H - e_S$) was determined for similar samples[5] to be below 0.03%, about three times smaller than the upper limit found here. Although our accuracy is limited, we find less than 3% of the strain expected for a pseudomorphic layer ~equal to the lattice mismatch of 0.04!. The accuracy of our strain analysis could be improved by measuring e below 100 K ~where the broadenings are smaller leading to more accurate CP energies!.

In conclusion, we have found that the optical constants ~refractive index and absorption coefficient! and their derivatives, related to band structure and transport parameters ~CP energies and broadenings!, of thick Ge layers on Si are virtually identical to those of bulk Ge. These results are in agreement with RHEED and EPD counts. Therefore, we should expect that electronic and optoelectronic devices fabricated using Ge on Si should have similar ~if not superior! characteristics compared to bulk Ge-based devices.

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