SECOND ORDER RAMAN SCATTERING OF CUBIC SILICON CARBIDE

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Abstract: Second order Raman scattering was measured on 3C-SiC free films prepared by chemical vapor deposition. Using the recently determined phonon dispersion of 3C-SiC from inelastic x-ray scattering and other data for phonon energies at critical points of the Brillouin zone, 2\textsuperscript{nd} order Raman features of 3C-SiC are well-defined and compared with theoretical calculation.

Silicon carbide (SiC) is currently being explored as a material for the next generation of high-power and high-temperature electronics and optoelectronics [1-2]. Cubic (3C) SiC is promising for these applications due to its special properties, such as large energy gap (2.2 eV at room temperature), high electric breakdown field, high saturation drift velocity, moderately high electron mobility, chemical inertness and temperature stability [3]. In recent years, great efforts have been made on the hetero-epitaxy and applications of 3C-SiC/Si materials and structures/devices. 3C-SiC is the only one among a large number (>150) of SiC polytypes that is achieved to grown on Si substrate, which can take the advantage of the strong Si semiconductor technologies for device fabrications. So far, chemical vapor deposition (CVD) and other techniques have been employed to successfully grow epitaxial crystalline 3C-SiC on Si [3]. The second order Raman scattering can give an insight into the lattice-dynamical properties and ultimately information on the strength and range of interatomic forces [4].

In this study, we present a 2\textsuperscript{nd} order Raman investigation on CVD 3C-SiC materials. Figure 1 shows a second order Raman spectrum from a CVD 3C-SiC free film (16 \(\mu\)m), which is similar to that Choyke reported first from Lely method grown small size single crystalline 3C-SiC [5]. Figure 2 shows the polarization behaviors of the first and second order Raman spectra from this 3C-SiC film.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{raman_spectrum.png}
\caption{Second order Raman spectrum from a CVD-grown 3C-SiC free film (16 \(\mu\)m).}
\end{figure}

Due to momentum conservation, the first order Raman modes can only be observed at the center of Brillouin zone (BZ), \(\Gamma\) point, for a perfect zincblende cubic SiC. The requirement of a net zero wavevector for two phonon states leads to the observable phonon overtones and combinations from \(\Gamma\), \(X\) and \(L\) symmetry points. The zone center TO and LO phonon frequencies (at \(\Gamma\)) have been determined from Raman measurements for bulk [6-8] and film [9,10] 3C-SiC. The frequencies for TO and LO phonons at L were known from the phonon dispersion curves along (111) direction.
deduced from phonon data of different SiC polytypes [6,8]. TO(X) and LO(X) values were obtained from PL measurements for 3C-SiC which has an indirect gap and conduction minima at X [11]. In particular, recent determination of the phonon dispersion on 3C-SiC by inelastic x-ray scattering has provided more reliable data of phonon energies at different critical points of the Brillouin zone of 3C-SiC. With these data, we can obtain all possible combinations of Raman phonon modes below 2000 cm\(^{-1}\). Our experimental Raman features at 1121, 1239, 1312, 1402, 1520, 1624, 1714, 1856 and 1896 cm\(^{-1}\) are assigned to two-phonon Raman scattering, as shown in Fig. 1. The strongest second order Raman phonon mode, located at 1520 cm\(^{-1}\), is assigned to 2TO(X). The second strongest two-phonon feature at 1714 cm\(^{-1}\) is close to TO(X)+LO(Γ). The intensities of the second order Raman features are more than one order of magnitude weaker than those of the first order phonons.

Theoretical calculations on the phonon density-of-states for SiC have been made [4,12-14]. In Refs. [12-14], SiC density-of-states up to 1000 cm\(^{-1}\) have been presented. Windl et al. [4] have calculated, using \textit{ab initio} phonon eigensolutions and phenomenological polarizability coefficients, the theoretical Raman spectra up to 2000 cm\(^{-1}\). Comparison of our experimental data with these calculations and discussion are underway.

![Figure 2. Polarization behavior of the first-and second-order Raman spectra from a CVD-grown 3C-SiC film.](image)

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