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Optical properties of 3C-SiC/Si (001) defect microstructures by exploiting Raman scattering and X-ray absorption fine structure measurements**Devki N Talwar**

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We report comprehensive studies of the optical and structural properties of microstructures in V-CVD grown 3C-SiC/Si (001) epilayers by exploiting Raman scattering and X-ray absorption fine structure measurements. By exploiting the phonon-assisted Raman scattering spectroscopy we have recognized the conventional optical modes $\sim 794\text{ cm}^{-1}$, 973 cm^{-1} and two additional phonon features near $\sim 625\text{ cm}^{-1}$ and 670 cm^{-1} - possibly falling between the forbidden gap of the acoustic and optical branches of 3C-SiC. Synchrotron radiation X-ray absorption fine-structure (SR-XAFS) measurements are performed by exploiting a double-crystal monochromator beamline at the National Synchrotron Radiation Research Center, Hsinchu, Taiwan. The measured X-ray absorption spectra are carefully examined to check the ability of experimental standards with the *ab initio* calculations. Temperature dependent profile of the unresolved $\sim 670\text{ cm}^{-1}$ Raman band indicates disordering by defects and/or stress that makes phonon lifetime shorter to instigate mode broadening. Accurate assessments of lattice dynamical, thermal and defect properties are achieved by exploiting phonons from a rigid-ion model fitted to the inelastic X-ray scattering data and expending apposite group-theoretical selection rules. Lattice relaxations around Si/C atoms attained by first-principles bond-orbital model for isolated defects have helped evaluating the necessary force constant variations to construct perturbation matrices of “complex-defect-centers”. For the isolated intrinsic C_{Si} and Si_{C} defects (T_d -symmetry) our methodical greens function (GF) theory predicted triply degenerate F_2 gap modes near $\sim 630\text{ cm}^{-1}$ and $\sim 660\text{ cm}^{-1}$, respectively. The GF simulations of impurity vibrations for a neutral “anti-site” $\text{C}_{\text{Si}}\text{-Si}_{\text{C}}$ pair (C_{3v} -symmetry) provided gap-modes to appear within the broad $\sim 670\text{ cm}^{-1}$ band at 664.8 cm^{-1} (a_1) and 660.6 cm^{-1} (e). These outcomes implying possible links of ASP defect to a proto-typical D_1 center in 3C-SiC are compared and deliberated against the existing experimental data.

Biography

Devki N Talwar, is a Distinguished University Professor in the Physics department at Indiana University of Pennsylvania (IUP), USA and conducts research on defects in semiconductor materials used in various electronics and optoelectronics applications. He has been with IUP for almost 29 years, and is the author of more than 130 refereed journal articles, four book chapters and more than 80 international conference presentations. He served as an Organizer in seven international conferences organized by Materials Research Society-USA, Singapore; 5th World Congress on Materials Science and Engineering-Spain, Optics, Mesoscopic Condensed Matter Physics, and Condensed Matter Physics-USA.

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