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Probing optical, phonon, thermal and defect properties of 3C-SiC/Si (001)

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Comprehensive results of theoretical calculations are reported to probe the optical, phonon, thermal and defect properties of 3C-SiC/Si (001). By exploiting Raman scattering (RS) spectroscopy we have recently recognized amongst the conventional optical modes ($\sim 794\text{ cm}^{-1}$, 973 cm^{-1}) in 3C-SiC, two extra phonons near $\sim 625\text{ cm}^{-1}$ and 670 cm^{-1} – possibly falling between the forbidden gap of the acoustic and optical branches. Accurate assessments of the 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 expanding appropriate group-theoretical selection rules. Lattice relaxations around Si/C atoms attained by the first-principles bond-orbital model for isolated defects in 3C-SiC has helped us evaluating the necessary force constant variations to construct perturbation matrices for intrinsic “complex-defect-centers”. For a nearest-neighbor “anti-site-pair” $\text{C}_{\text{Si}}\text{-Si}_{\text{C}}$ defect, our methodical Greens function simulations of the gap modes have provided not only a strong support to the observed phonon features of DI-center but also afforded validation for a broad band observed near $\sim 670\text{ cm}^{-1}$ in RS experiments.

Biography

Devki N Talwar graduated from Allahabad University in India in 1976 with a PhD degree in Condensed Matter Physics. From 1977-80, he worked as a Visiting Scientist at the Commissariat a l'Energie Atomique, Saclay, Gif-sur-Yvette, France with Professor M. Vandevyver. While at Saclay he collaborated with theoretical / experimental group of Professor M. Balkanski, including Karel Kunc, M. Zigone, and G. Martinez and supervised 3 PhD theses. In January 1980, he joined the Physics Department, University of Houston as a Visiting Professor and collaborated with Professor C. S. Ting on problems related to the electronic properties of defects in Semiconductors and supervised a PhD student. From 1982-87, he was a faculty at Texas A&M University. He joined the Physics Department at Indiana University of Pennsylvania in 1987, supervised 20 MS theses. Since 2007-2014, he served as a Chairperson of the Physics Department.

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