Scattering tensors and optical transitions in Si and Ge

H. W. Kunert^{**,1}, A. G. J. Machatine^{*,1}, P. Niyongabo¹, M. Govender^{1,2}, and B. W. Mwakikunga²

1 Department of Physics, University of Pretoria, Pretoria 0002, South Africa 2 CSIR National Centre for Nano-Structured Materials, P. O. Box 395, Pretoria 0001, South Africa

* Corresponding author: e-mail augusto.machatine@up.ac.za

** e-mail herbert.kunert@up.ac.za

Abstract

The selection rules (SR's) for the Kronecker product (KP) of Si and Ge irreducible representations (irreps) are required to determine the intervalley scattering processes. The SR's for transitions between the lowest conduction band minima at \int , X and L high symmetry points and the highest maximum of the valence band (VB) in the Brillouin zone of $_{7h}$ O space group symmetry are determined. The symmetry of phonons due to electron-phonon (EI-Ph) interaction follows from the KP's: $L_1 \otimes \int_{12} (\int_{2^-}), \Delta_1 \otimes \int_{12} (\int_{2^-}), L_1 (L_{1+}) \otimes \Delta_1$ for Ge and $L_1 \otimes \int_{15} (\int_{4^-}), \Delta_1 \otimes \int_{15} (\int_{4^-}), L_1 (L_{1+}) \otimes \Delta_1$ for Si. The elements of EI-Ph scattering tensors are linear combinations of the Clebsch-Gordon coefficients (CGC's). Here we have computed the coupling coefficients relevant to scattering tensors. Our theoretical results confirm the available experimental data.