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LATTICE VIBRATION AND LATTICE DILATION EFFECTS IN THE TEMPERATURE DEPENDENCE OF THE SILICON ENERGY GAP

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ABSTRACT

A theoretical calculation using potential scaled orthogonalized plane wave (PSOPW) method was used and implemented to predict the effect of lattice vibration and lattice dilation in the temperature dependence of the fundamental energy gap for Si. Through the calculation of the maximum of valence band and minimum of conduction band at different temperatures, the effect of temperature on the energy gap for lattice vibration (electron-phonon interaction), lattice dilation (thermal expansion) and total effect were calculated separately using the computer Pascal code PSOPW. The calculation for the temperature dependence of the band gaps predict the contribution of lattice vibration dependence of the energy gap is more than that of lattice dilation and the rate of change of valence band with temperature is more than that of the conduction band.

Keywords: Energy Gap; Energy band; LV; LD; LDV

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