The study outlined in this dissertation elucidate the thermal and structural properties of ZrB$_2$ based ceramics as choice materials for high temperature applications. Thermal properties were investigated to improve understanding on aspects that are affected by point defects and impurities at nanoscale and electron level using a combination of lattice dynamics, molecular dynamic (MD) simulations and density functional theory. Macroscopic approach to heat transfer is limited as characteristic time and length scale reduces and become analogous to phonon relaxation times and mean free path over the stages transfer. A correlation between atomic structure property and thermal parameters were investigated using phonon (lattice vibration) analysis. In this study is described thermal contribution in a collaborative effort to develop a defect-adaptive predictive model for zirconium diboride (ZrB$_2$) properties. This portion focuses on the thermal property of point defects and impurity defects of metallic and covalent form. Introduction of defects into perfect ZrB$_2$ to tune or investigate the variations in its thermal conductivity, expansivity and heat capacity for desired application provides endless space for controllable parameters. Green-Kubo (GK) method which is well established in the study of transport phenomena was applied to compute thermal transport with expected differences in heat current in the various axial directions. It relates the thermal conductivity of solids to the integral of autocorrelation of heat current within the lifetime of the fluctuations. Evolution in the microstructure of ZrB$_2$ under thermal stress was studied. Temperature dependency of the coefficient of thermal expansion (CTE) and anisotropy observed in the elongation of lattice parameter of ZrB$_2$ were presented. Lattice vibration also characterizes the capacity for materials to store thermal energy storage. Phonon-based constant volume heat capacity trend with temperature is shown in the presence and absence of impurities (C, Si, Hf, W). The energy level changes in the valence and conduction region due to impurities were characterized. Calculations of total and projected density of states using density functional theory (DFT) to understand atomic level variation are shown and compared to phonon dispersion. Dynamic stability of structures in the presence of covalent and metallic impurities were correlated to the imaginary and non-imaginary modes of phonons.