List of Figure Captions

Figure 1. Comparison of the density of states as a function of energy obtained ab initio to the density of states for a parabolic approximation to the valence and conduction bands.

Figure 2. Calculated values of $E_F$ as a function of temperature for three different density of states approximations in the intrinsic (upper three curves) and heavily doped (bottom three curves) regimes. The dashed lines corresponds to $E_F$ using the ab initio density of states, the solid lines are determined with Green’s $N_C$ and $N_V$ and the dotted lines were obtained with the $T^{3/2}$ using the data from Sze.

Figure 3. Comparison of calculated dopant enhanced solubility of Fe in Si as a function of temperature using different density of states approximations while assuming $E_T$ remains at a constant fraction of $E_G$. The doping level is $N_A=1.5\times10^{19}$ which corresponds to the doping level of the Si investigated by McHugo et al (solid squares denote their data points). With the exception of the fine dotted line, all calculations were performed using Fermi-Dirac statistics to calculate $E_F$. A comparison between the fine dotted line ($E_F$ obtained with the Boltzmann approximation for the $T^{3/2}$ model) and the dashed double dot line illustrates the error generated using the Boltzmann approximation. The solid line represents the intrinsic Fe solubility.

Figure 4. Comparison of calculated dopant enhanced solubility of Fe in Si for different temperature dependencies of $E_G$. $E_T$ was held a constant fraction of the gap and we use the $T^{3/2}$ model for effective density of states. The dashed line was calculated using the Varshni relation for $E_G$ with the parameters of Alex et al while the dotted curve calculation relies on the extrapolation of a semi-empirical model for $E_G$.

Figure 5. Comparison of calculated dopant enhanced solubility of Fe in Si for different temperature dependencies of the Fe defect level, $E_T$, in the gap. Dotted line was calculated assuming that $E_T$ is a constant distance from the valence band edge. For the dot-dashed curve, $E_T$ was held a constant fraction of the gap. The dashed curve was obtained by assuming that $E_T$ is a constant distance from the conduction band edge. The solid line denotes intrinsic solubility.