

Figure 1

PMMT model without defect sites (solid lines) v.s. experimental sticking coefficient (dots), direct dosing. Although high temperatures (above 700K) fits fairly well, the model fits poorly at lower temperatures.

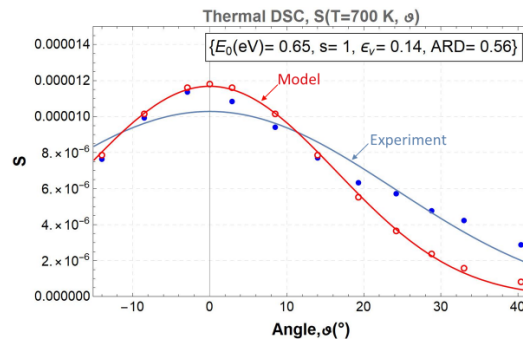


Figure 2

PMMT model without defect sites (red) v.s. experimental sticking coefficient (blue dots) at $T_g=T_s=700K$, angular distribution. Fitting is acceptable at small angles, discrepancy gets bigger at big angles.

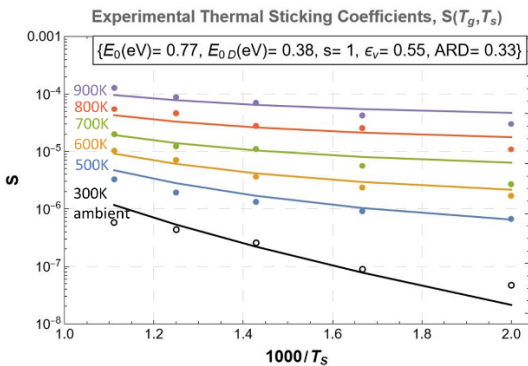


Figure 3

PMMT model with defect sites v.s. experimental. Agreement is good across all temperatures in question, even for 300K ambient dosing.

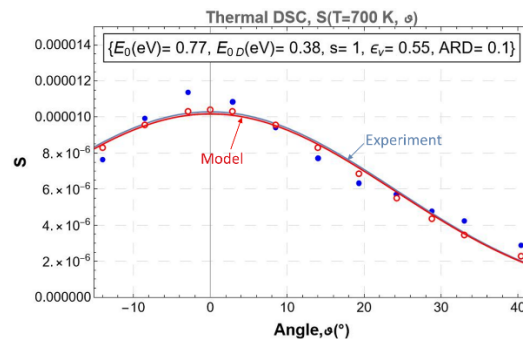


Figure 4

PMMT model with defect sites (red) v.s. experimental sticking coefficient (blue dots) at $T_g=T_s=700K$, angular distribution. Solid blue line is the numeric fitting to experimental data. Model and experiments agree well.

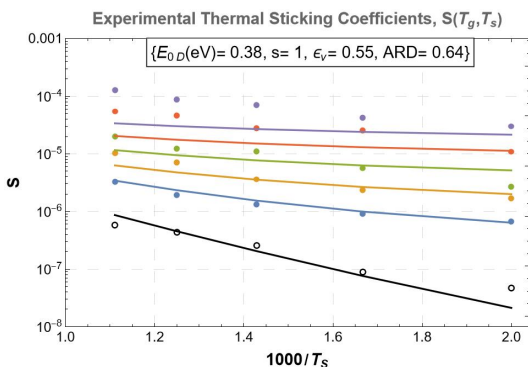


Figure 5

PMMT model showing only the defect sites activity. At low temperature, defect sites play a significant role in promoting C-H bond cleavage in methane.