

Supporting Information

Impact of Angular Deviation from Coincidence Site Lattice Grain
Boundaries on Hydrogen Segregation and Diffusion in α -iron

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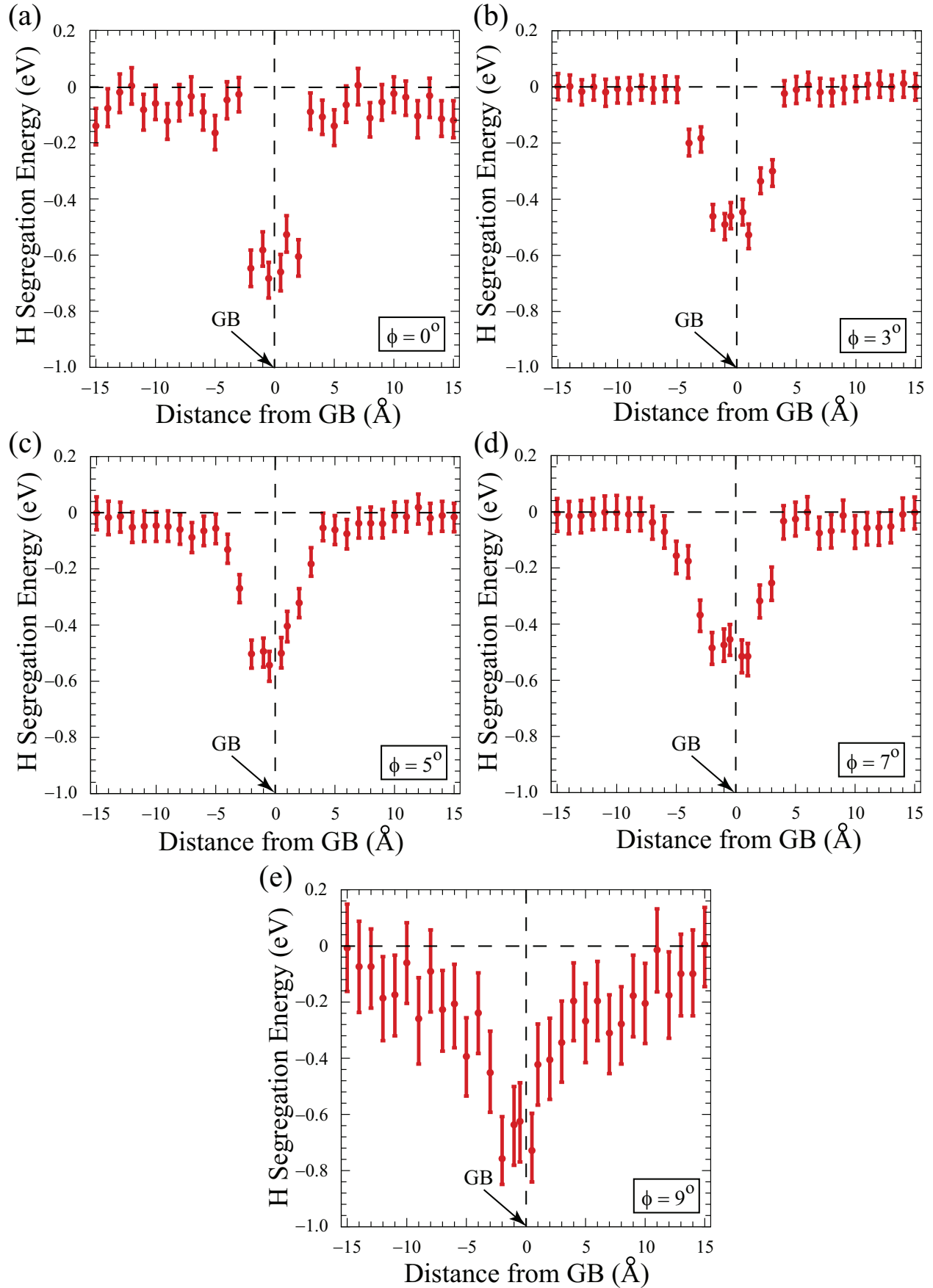


FIG. S1: The H-segregation energy as a function of position from the GB for (a) ideal $\Sigma 3$ (111) $[\bar{1}\bar{1}0]$ GB; (b) $\phi = 3^\circ$; (c) $\phi = 5^\circ$; (d) $\phi = 7^\circ$; and (e) $\phi = 9^\circ$. The symbols represent the average values based on statistical analysis and mean estimation with a 95% confidence interval, and the error bars represent the standard deviation.

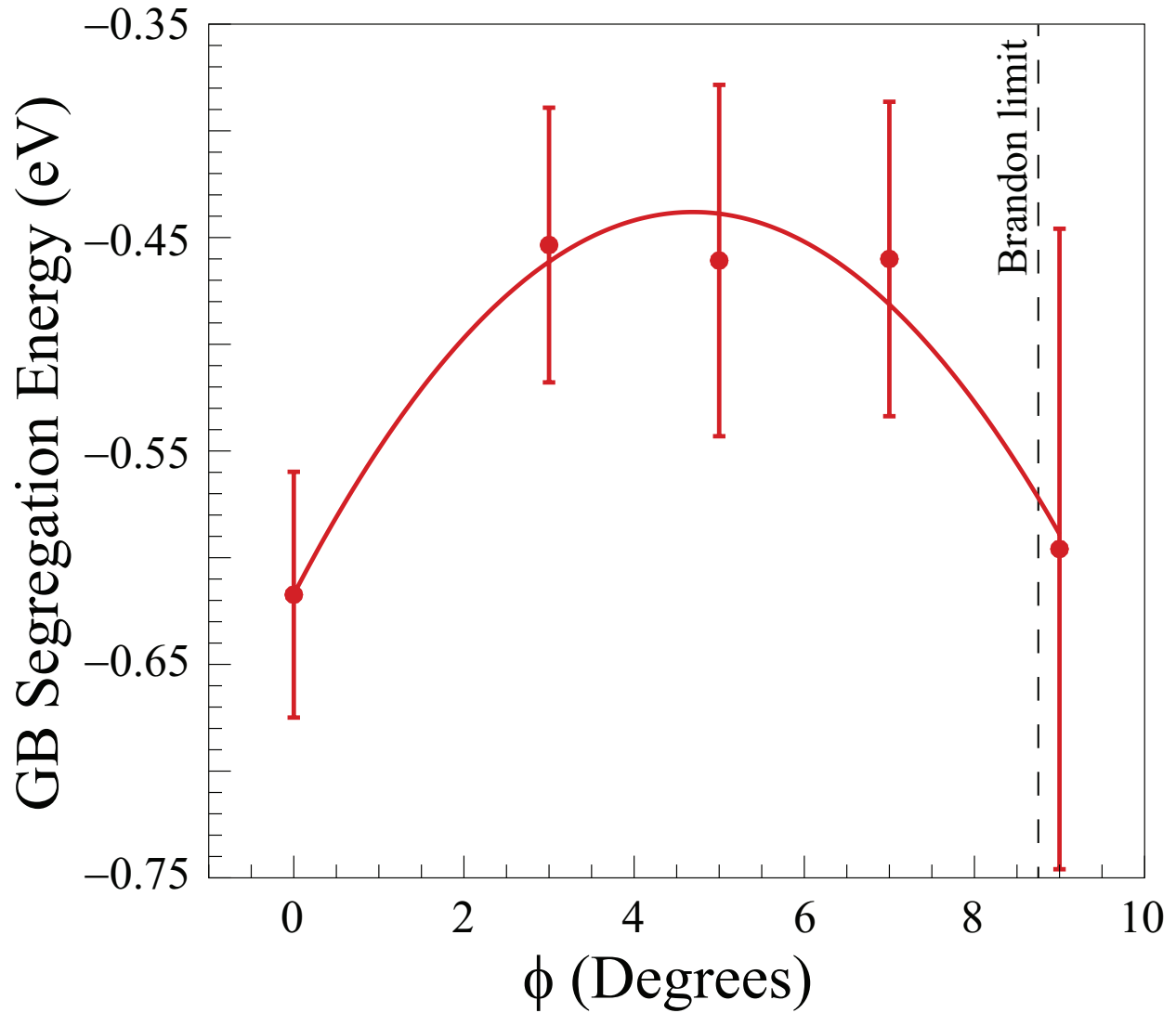


FIG. S2: The H-segregation energy within a 2 \AA layer encompassing the GB as a function of the deviation angle from the ideal $\Sigma 3$ (111) $[\bar{1}\bar{1}0]$ GB. The symbols represent the average values based on statistical analysis and mean estimation with a 95% confidence interval, the error bars represent the standard deviation, and the solid line represent the best curve fit.

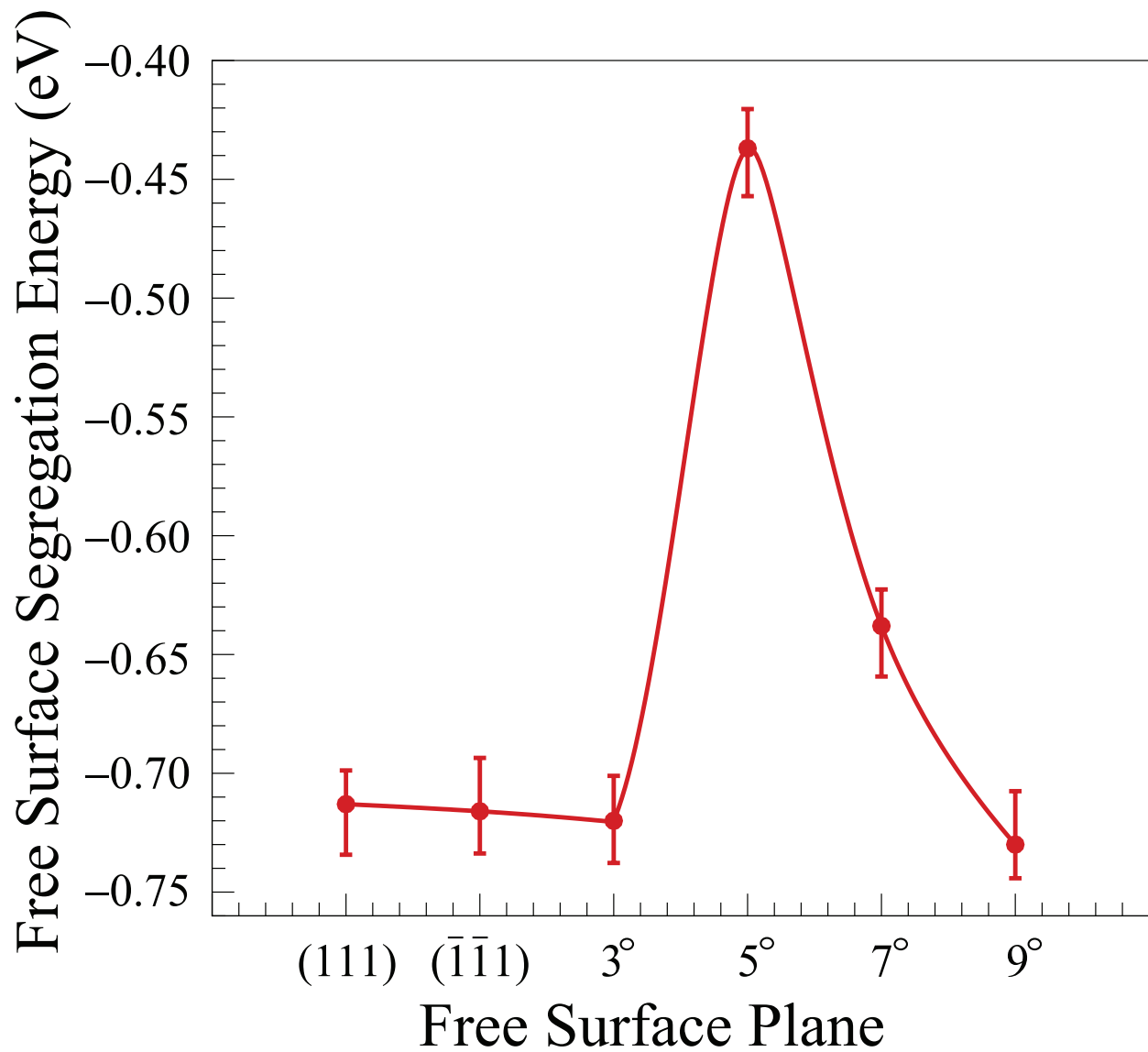


FIG. S3: The free surface H-segregation energy in both grains and as a function of deviation angle from the $\Sigma 3$ (111) ideal symmetry plane. The symbols represent the average values based on statistical analysis and mean estimation with a 95% confidence interval, the error bars represent the standard deviation, and the solid line represent the Akima interpolation fit.