The solid lines in Fig. 6 represent the least square fits of the MD data for $P(w)$ to the disjoining-potential formulas given by Eqs. 7, 1 and 2 for the $\Sigma 9$ twist boundary, and Eqs. 7, 1 and 3 for the $\Sigma 9$ tilt boundary. For the $\Sigma 9$ twist boundary the potential parameters obtained from the separate fits to the data for the individual temperatures span the range δ=0.25 to 0.29 nm, and $\Delta\gamma$=101 to 150 mJ/m^2. For the $\Sigma 9$ tilt boundary the fitted values for δ_1 and δ_2 ranged between 0.142 to 0.144 and 0.143 to 0.144 nm, respectively, $\Delta_1 - \Delta_2$ spanned the values 103 to 163 mJ/m^2, and Δ_2/Δ_1 took values between 1.003 and 1.006. With these fitted potential parameters, the disjoining potential for the $\Sigma 9$ tilt boundary exhibits a weak minimum at a width w_m with values ranging between 0.32 and 0.36 nm, and a depth relative to $2\gamma_{SL}$ varying between -7 and -11 mJ/m^2. The fact that the MD calculated width histograms can be accurately described by disjoining potentials with a relatively narrow range of fitted potential parameter values indicates that the formalism described in the previous section represents a valid model for describing the temperature dependence of the structural disorder observed in these boundaries.

In order to refine the calculation of the disjoining potential for the $\Sigma 9$ twist and tilt boundaries, we employ the histogram analysis described in the previous section, involving a refinement of both the shift parameters a_i and the potential parameters in Eqs. 2 and 3 for the twist and tilt boundaries, respectively. The resulting fits are shown in Fig. 7 and correspond to the following values for the potential parameters: $\delta = 0.25$ nm and $\Delta\gamma = 156$ mJ/m^2 for the $\Sigma 9$ twist boundary, and $\Delta_1 - \Delta_2 = 103$ mJ/m^2, $\Delta_2/\Delta_1 = 1.003$, $\delta_1 = 0.1471$ nm, $\delta_2 = 0.1474$ nm for the $\Sigma 9$ tilt boundary. These parameter values are consistent with the values given above from the independent fits. The excellent agreement of the fits with the MD data in Fig. 7 again indicates that the disjoining-potential formalism represents an accurate framework for modeling the premelting behavior of these $\Sigma 9$ boundaries. The analysis used to obtain the results in fits in Fig. 6 assumed a melting point of $T_M = 1710$ K. If the melting temperature is changed even by one degree,i.e., $T_M = 1709K$ then poor fits to $P(w)$ are obtained for the data at the lowest undercoolings.

The calculated disjoining potentials in Fig. 7 are characterized by the following features. For the $\Sigma 9$ tilt boundary the disjoining potential has a minimum at a finite width, w_m ,which corresponds to the average equilibrium grain boundary width at the melting temperature. The potential is repulsive for $w < w_m$ and attractive for $w > w_m$. In contrast, the $\Sigma 9$ twist boundary features a purely repulsive disjoining potential that is well modeled by exponential