Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Support information

Table S1 The constructed Li_3OCl GB supercell dimensions

Structures	Lattice parameters (Å)
Σ3(111)	a=5.53, b=5.53, c=54.18
Σ3(112)	a=5.53, B=6.77, c=57.46
Σ5(210)	a=3.91, b=8.74, c=52.46
Σ5(310)	a=3.91, b=12.36, c=49.46

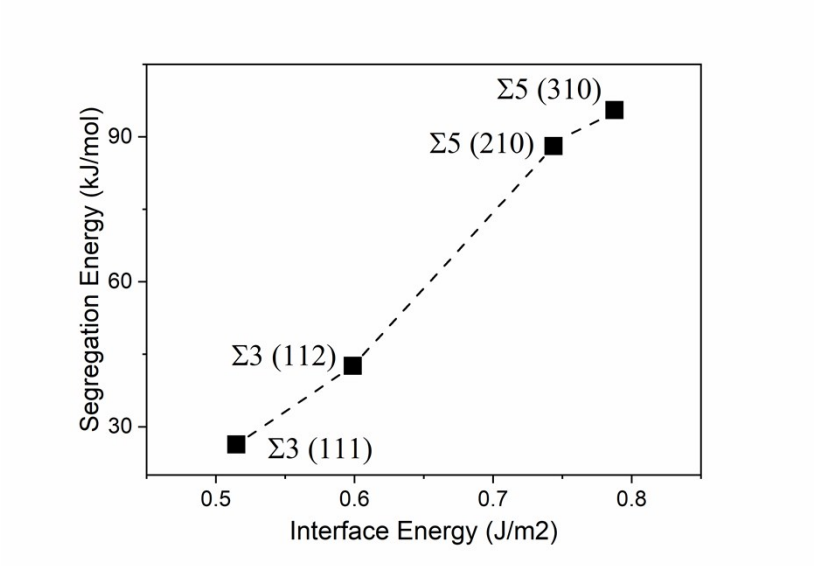

Figure S1 The relationship between segregation energy and interfacial energy for Σ3(111), Σ3(112), Σ5(210) and Σ5(310), where the Li vacancy segregation energy is the chosen as the lowest in each GB structures

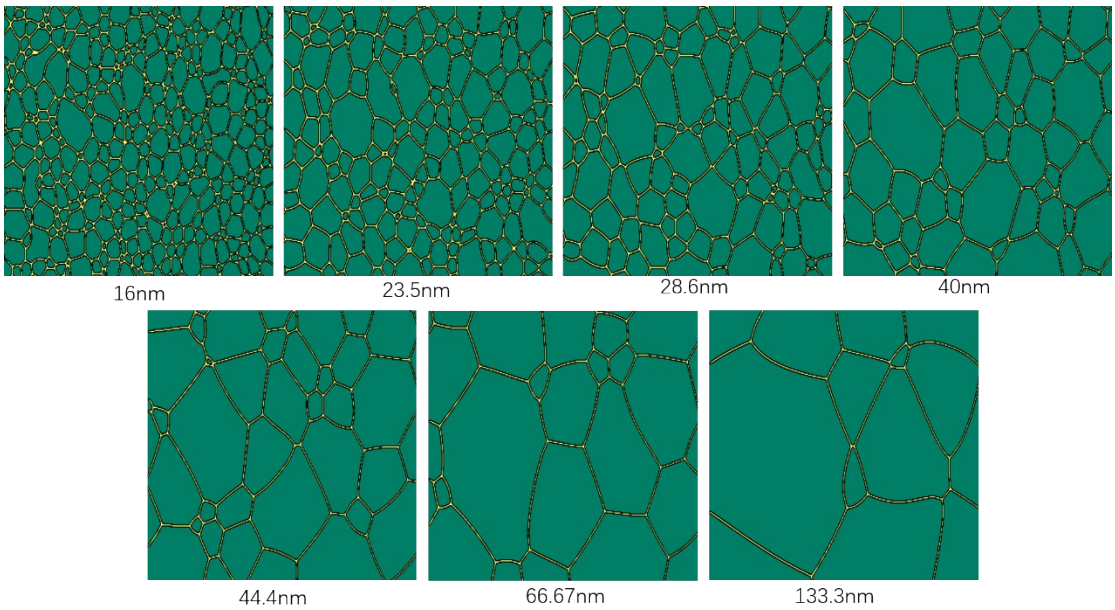

Figure S2 *The Li vacancy distribution in polycrystalline Li3ClO with different grain sizes with segregation*