Electronic Supplementary Material (ESI) for Nanoscale.

Supporting information

Grain boundary phases in bcc metals

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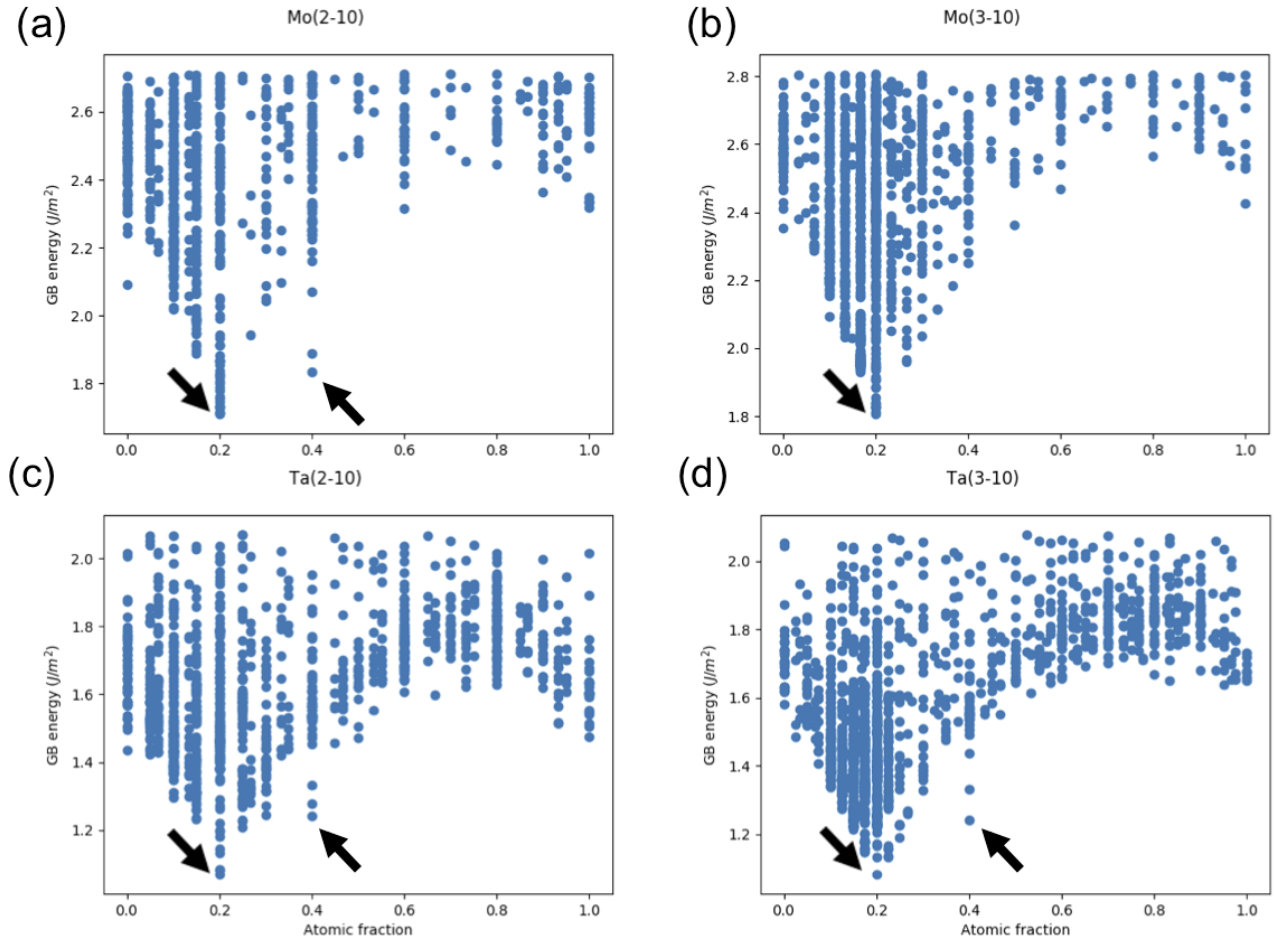

Fig. S1. Results of the evolutionary search for $\Sigma 5(001)$ (210)-twist and (310)-twist boundaries in Mo (a and b) and Ta (c and d). GB energy is plotted as a function of the number of atoms [n]. The arrows indicate different GB phases at [n]=1/5 and [n]=2/5.

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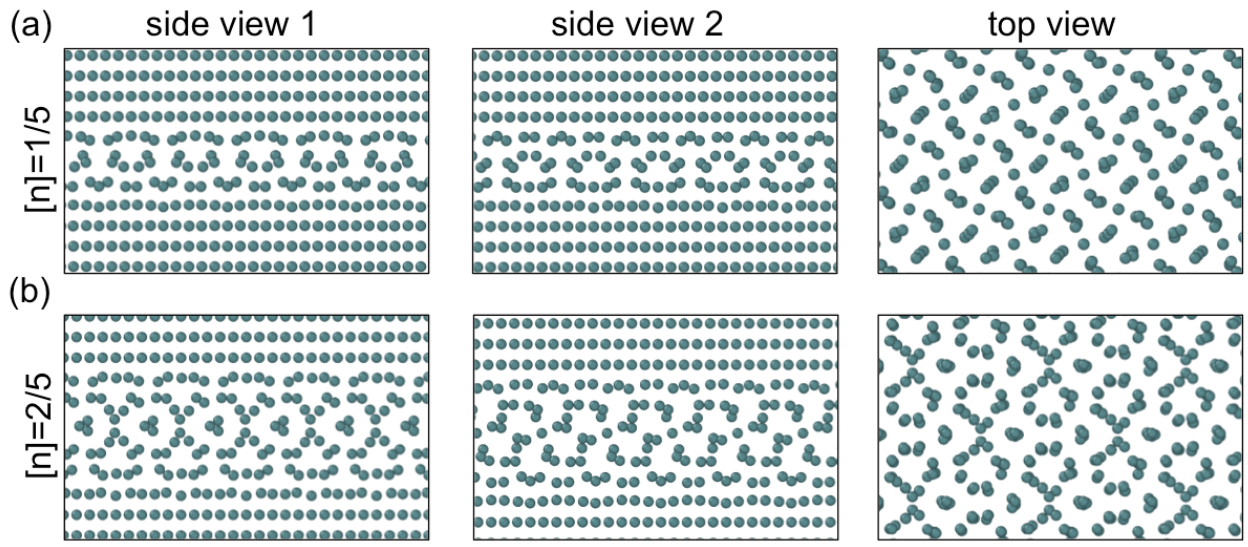

Fig. S2. Lowest energy structures at [n]=1/5 and [n]=2/5 of the $\Sigma 5(001)$ (210)-twist boundary predicted by the evolutionary search in W, Mo and Ta.