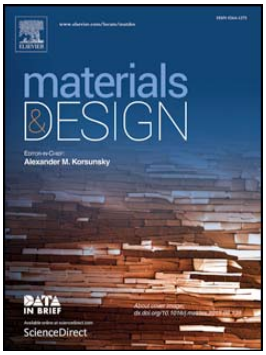

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Symmetrical tilt grain boundary engineering of NiTi shape memory alloy: an atomistic insight

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Abstract

The role of austenitic symmetric tilt grain boundaries (STGBs) on the martensitic transformation in NiTi alloy during thermal cycling between 500 K and 10 K are studied from molecular dynamics simulations. Four austenitic STGBs including $\Sigma3[1\bar{1}0](111)$, $\Sigma3[1\bar{1}0](112)$, $\Sigma9[1\bar{1}0](114)$ and $\Sigma9[1\bar{1}0](221)$ have been considered. Through martensitic transformation, the austenitic STGBs transform to martensitic grain boundaries (GBs) and martensitic twin boundaries form in the interior of the simulation models. After austenitic transformation, the martensitic GBs recover to the austenitic STGBs and the twin boundaries disappear. We find that the roles of STGBs on the martensitic transformation can be divided into three groups based on the martensite start temperature (M_s). (1) The $\Sigma3[1\bar{1}0](112)$ and $\Sigma9[1\bar{1}0](221)$ STGBs retard the martensitic transformation, i.e., decreases

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