Atomic scale processes of phase transformations in nanocrystalline NiTi shape-memory alloys
6. Summary and conclusions

Large-scale MD simulations have been performed to provide an atomic scale understanding of phase transformations in nanocrystalline NiTi shape-memory alloys. The present simulations faithfully reproduce the various experimentally reported characteristics of the phase transformations in nanocrystalline NiTi related to the over-stabilization of the austenite phase. The simulations further provide detailed insights into the atomic scale processes of the phase transformations. During the austenite-to-martensite transformation, the martensite phase nucleates in the grains’ interior and grows towards grain boundaries. The resultant martensite phase is characterized by a unique nanotwinned structure with multiple domains. During the martensite-to-austenite transformation, the austenite phase nucleates at grain and domain boundaries and grows towards the grains’ interior. In nanocrystalline NiTi with very small grains, a considerable amount of irrecoverable strain is observed during the stress-induced phase transformation. Our work clearly reveals that the irrecoverable strain results from a plastic deformation at the grain boundaries and that a pre-training under cyclic loading can greatly reduce this strain. By comprehensively analyzing experimental information and our results, a unified governing mechanism is proposed for the characteristics of both temperature- and stress-induced phase transformations in nanocrystalline NiTi.