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Structure of Grain Boundaries in α-Zirconium and Niobium

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Abstract : Due to superior mechanical, creep and nuclear cross section, zirconium and niobium (Zr-Nb) based alloys are commonly used as nuclear materials for the manufacturing of fuel cladding and pressure tubes in nuclear power plants. In this work, symmetrical tilt grain boundary (STGB) structures in α-Zr are studied for their structure and energies along two tilt axes- [0001] and [0-110] using MD based simulations. Tilt grain boundaries are obtained along [0001] tilt axis, and special twin structures are obtained along [0-110] tilt axis in α-Zr. For Nb, STGBs are constructed along [100] and [110] axis using atomistic simulations. The correlation between GB structures and their energies is subsequently examined. A close relationship is found to exist between individual GB structure and its energy in both α-Zr and Nb. It is also concluded that the energies of the more coherent twin grain boundaries are lower than the symmetrical tilt grain boundaries.

Keywords : grain boundaries, molecular dynamics, grain boundary energy, hcp crystal
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