Influence of Mn on Plastic Deformation in Polycrystalline α-Ti–Mn Alloys

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Titanium alloys are widely used in aerospace, biomedical, and energy applications owing to their high specific strength, corrosion resistance, and biocompatibility. In order to investigate the influence of the manganese on the mechanisms of plastic deformation in polycrystalline α-phase Ti-Mn alloys we have performed a series of molecular dynamics simulations for uniaxial tensile tests at 300K and $10^9 s^{-1}$ strain rate for Ti-2at%Mn, Ti-4at%Mn, as well as pure Ti and analyzed the results.

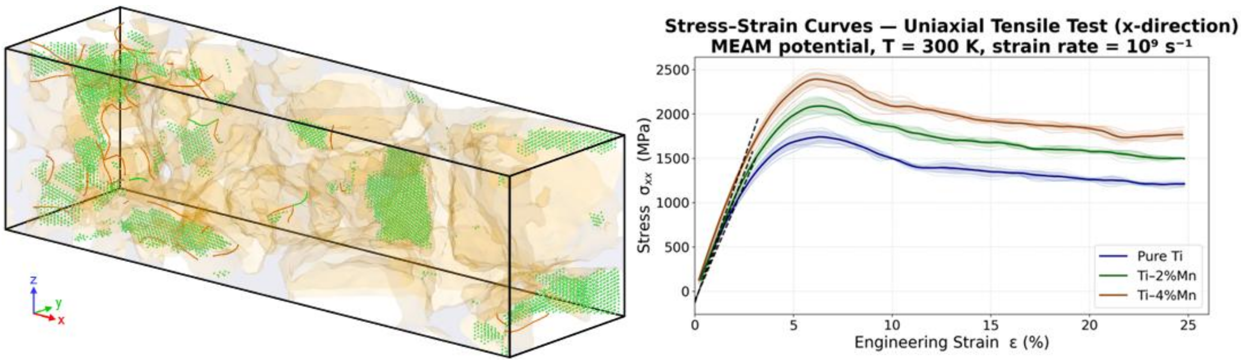

Figure 1. Example of simulated cell after tensile test, as well as stress-strain curves for pure Ti, Ti–2Mn and Ti–4Mn.

In pure Ti, plastic deformation is mediated mainly by the growth of the grain boundaries, reaching 56at% at the end of strain test, compared to 46% in Ti-2Mn and 39% in Ti-4Mn at.%. Apart from the grain boundary growth, a different mechanism of deformation is occurring inside the grains. When strain is applied, stacking faults are formed (which in HCP material are planes ordered as FCC), limited inside the grain by the 1/3<1-100>-type edge dislocations, or by the grain boundaries. Under further application of strain, three different options are possible. (i) Two 1/3<1-100>-type dislocations surrounding a stacking fault form one 1/3<11-20>-type dislocation, that is terminated on the grain boundaries, following the balance of energies, e.g. 1/3[-1010]-1/3[1-100]=1/3[-2110]. This leads to a decrease in the percentage of FCC atoms. (ii) Stacking fault is absorbed into the grain boundary, leading to a decrease in the density of 1/3<11-20>-type dislocations. (iii) Stacking faults grow until they fully terminate on the grain boundaries and either stabilize or split the grain in two. Stacking faults form in every sample of every alloy, but in alloys with Mn, their number and size are increased. As such, a clear trend is observed: increasing Mn content leads to higher resistance to deformation, as reflected in the stress–strain response. At the atomic scale, plastic deformation is governed by dislocation nucleation and their subsequent interactions. The addition of Mn modifies the local atomic environment, hindering dislocation mobility and contributing to the observed strengthening.

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