Influence of Interstitial Impurities on the Griffith work in Ti-based Alloys

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It is known that segregated impurities can induce embrittlement of materials. For example, even small concentration of H reduces the mechanical strength and may limit some industrial applications of advanced materials. In order to understand the grain boundary (GB) cohesion it is necessary to find general rules for the description of the relationship between microscopic features and macroscopic material properties. In this work we investigate the influence of the interstitial (H, B, C) and substitutional (Co, Ni, Pd, Al) impurities on the chemical bonds at the GB and surface in the series of the B2-TiMe alloys, where Me=Fe, Co, Ni, Pd. The atomic and electronic structures of TiMe alloys with Σ5(310) GB and (310) surface were investigated by the plane-wave pseudopotential method. The change of the Griffith work (GW) due to an interstitial impurity was calculated as the difference in GW for impurity doped and undoped systems or the difference between segregation energies of the impurity to surface and GB. The influence of impurities on H sorption properties was also studied. It was shown that hydrogen sorption energies at the grain boundary and surface depend strongly on the H local environment. The most preferential sites for both B and C segregation are the same as for H. The analysis of the electronic properties allows us to establish the microscopic nature of the chemical bonding of interstitial impurities at the interfaces. It was found that H decreases the surface energies more significantly than the GB energy, which results in decrease of the Griffith work and indicates also the decrease of the strength of the grain boundary. The segregation of H at the GB makes intergranular fracture much easier because the bonding between metal atoms, which are neighbors of H, is weakened. In contrast to H other impurities (B or C) lead to opposite effect on the Griffith work. Our estimation of the Griffith work for the alloy containing both B and H atoms gives its increase in comparison with undoped alloy but the effect of carbon on the GB strengthening during hydrogenation seems to be negligible. The contributions of the chemical and elastic mechanisms to the binding energies and GW are discussed.