Surfaces and Interfaces

The effects of quaternary alloying additions on the TiAl alloy: Preferential site occupancy, interfacial energetics to physical parameters

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Abstract
The effect of Nb, Sn, Mn, and Si at a concentration of (0.3-2 at. %) on -TiAl based alloys' preferential occupancy, interfacial energetics and mechanical properties were investigated by density functional theory (DFT) encompassed by the typical gradient estimation configuration and substantiated by experimental work. The site occupancies, elastic constants, shear and bulk modulus, B/G ratio, Poisson's ratio, hardness and universal anisotropy are systematically elucidated. The results indicated that Mn adamantly occupies Ti sites, while the Nb, Sn and Si occupy Al sites, with no significant influence on the alloy composition in-terms of their site preference. Interfacial energy of /a2-M system is the prerequisite energy to generate an interface from bulk materials. The stability criteria were satisfied attributable to Cij's values greater than zero. The overall mechanical properties of the substitutional solid solution-TiAl alloy exhibited improved ductility. The alloy was produced by vacuum arc melting, with subsequent annealing to achieve homogeneity. The TEM results demonstrated that the a2/ interface boundaries yielded the -TiAl {111} <110>||a2-Ti3Al (0001) <110> orientation relationship.