A Study on the Twinning Energy for NiTi Alloys using First Principles Calculations

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In order to study the twinning behavior of shape memory alloys, we performed the density functional theory calculations within a local density approximation. We modeled a NiTi structure consisted of two detwinned martensite crystals and a twinned (001) plane between them. The lattice parameters and elastic constants of stable structures were obtained for the twinned martensite phase. By comparing with detwinned ones, we calculate the twinning energy and the required stress to make twinning. In addition, the effect of the distance between two parallel twin planes on the twinning energy was investigated.

Keywords: Twin, NiTi, DFT, Twinning Energy