7th ECCOMAS Thematic Conference on Smart Structures and Materials
SMART 2015
A.L. Araújo, C.A. Mota Soares, et al. (Editors)

Abstract ID-018

AN INVESTIGATION ON THE CRYSTAL STRUCTURES OF TI50NI50-XCUX SHAPE MEMORY ALLOYS BASED ON DENSITY FUNCTIONAL THEORY CALCULATIONS

Liangliang Gou, Yong Liu, Teng Yong Ng

School of Mechanical and Aerospace Engineering, Nanyang Technological University, Singapure
LGOU1@e.ntu.edu.sg ; MLiuY@ntu.edu.sg ; MTYNg@ntu.edu.sg

Keywords: Shape-Memory Alloys, Density Functional Theory, Phase Transformation, Electronic Structure, Phase Stability

Summary: The present research has investigated the martensite crystal structures and electronic structures of Ti50Ni50-xCux (x = 0, 5, 12.5, 15, 18.75, 20, 25) shape memory alloys using density functional theory (DFT). It is found that with Cu addition to NiTi, the lattice parameters (a and c) and the monoclinic angle decrease, whereas the lattice parameter b increases. When Cu content is increased to around 20 at%, an orthorhombic crystal structure is formed which agrees well with reported experimental observations. In particular, by introduction of Cu atoms into TiNi martensite crystal, Ti and Ni/Cu atoms move significantly along x-axis but insignificantly along y-axis and z-axis for all alloys examined. As a result, the distance between two Ni/Cu atoms increases while the Ti atoms get closer along x-axis, which is responsible for the decrease in the monoclinic angle. With increasing Cu content, fewer electrons were transferred from Ti to Ni in comparison with that in binary NiTi alloys, leading to a weaker interaction between them, which results in an increase of bond length. As the movements of both Ti and Ni/Cu atoms along x-axis are continuous, the monoclinic angle decreases gradually without dramatic change.