11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

THE STUDY ON SHAPE MEMORY PROPERTIES OF NI-AL ALLOYS BY MOLECULAR DYNAMICS SIMULATION

I-Ling Chang[1]*, Chin-Chen Hsu[1] and Ta-Hsiung Chao[1]

[1] Department of Mechanical Engineering, National Cheng Kung University, No. 1 University Road, Tainan, 70101 Taiwan, ilchang@mail.ncku.edu.tw

Key Words: *Shape Memory Alloy, Martensite, Austensite, Phase Tranformation Temperature.*

We employed molecular dynamics simulation to investigate the shape memory properties of Ni-Al alloy bulks. The effects of Ni composition ratio and the simulated crystal orientation on phase transformation were studied. At low temperature, different loading conditions were applied to the alloy bulk till plastic deformation is observed. Then, the deformed bulk went through the temperature cycle to examine whether it would restore to the original shape.

From the simulation, we found that Ni-Al is body-centered cubic structure (austensite) at high temperature and transforms to martensite phase at certain temperature, except for the one with 50% Ni composition ratio. The phase transformation temperature was affected by the Ni composition ratio. It was observed that different simulated crystal orientated models, which possess the same Ni composition ratio and atomic arrangement in space, would have the same phase transformation temperature. And the deformations of different crystal orientated models at various temperatures could be described using coordinate transformation relation. For the same model under different loading conditions, it was found that not every plastically deformed model would restore to its original shape after the thermal cycle. With the assist of slip vector, only those were loaded to slip along <110> direction would exhibit shape memory behavior. For those loading which would restore to its original shape, the corresponding maximum shear stress was noticeably smaller than those did not restore.