



Contribution ID: 353

Type: **Poster**

A theoretical study of Ni segregation through NiTi/tio₂-x

Tuesday 19 June 2018 18:00 (20 minutes)

The Nitinol (acronyms for NiTi Naval Ordnance Laboratory) is quasi equiatomic alloy of Ni-Ti known for its properties of shape memory, superplasticity, strength and biocompatibility. It is the most widely used form memory alloy in the production of biomedical devices. However, the presence of Ni in metallic or oxidized form on its surface or the release of it from the core of the alloy is a serious problem because of its allergenic properties and toxicity to human tissue. The most usual procedure is the modification of the surface by a coating that resists corrosion and is biocompatible. The simplest of the procedures consists of a surface oxidation that manages to grow an oxide film on the NiTi, the Ti being oxidized preferentially. For this reason we performed a DFT study of Ni segregation for different oxide coverage. Our results show that Ni diffusion is strongly dependent of the presence of Ti and o vacancies and the nature of an intermediary oxidation layer. We also analyzed the changes in the electronic structure and bonding at the interface.

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Session Classification: Poster Session Tuesday

Track Classification: Surface Science & Applied Surface Science