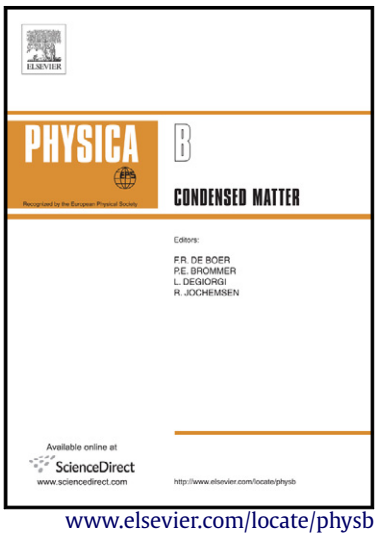

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First-principles investigations of oxygen adsorption at TiNi surface and the TiO_2/TiO – TiNi interface

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Abstract. *Ab-intio* study of the interaction of atomic and molecular oxygen with the TiNi(110) surface were performed using the projector augmented wave method with generalized gradient approximation for the exchange-correlation functional. The oxygen adsorption energies were calculated and the preferential adsorption sites of oxygen atom on the surface were determined. Our results confirmed the formation of a Ni-rich layer at the alloy-oxide interface. Atomic and electronic structure of both TiO/TiNi(110) and TiO_2/TiNi(110) interfaces were analyzed. The formation energies (E_f) of point defects at the interfacial layers as well as in bulk TiNi, monoclinic TiO, and rutile TiO_2 were estimated. It was shown that E_f of Ti-Ni swap defect has a lower energy than that for the Ni antisites at the TiO_2(100)/TiNi(110) interface. In the case of TiO(100)/TiNi(110) interface, the formation energies of Ti-Ni swap and Ni-antisites defects are close to each other. Our results demonstrated that E_f of Ni-defect in TiO is twice less than that in TiO_2. The increase in the formation energies of defects in TiO_2 reveal the increase in diffusion barriers of Ni atoms in comparison with those in oxides with a lower oxygen content, which hampers Ni segregation.

Keywords: electronic structure, TiNi, oxidation, interface, defects

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