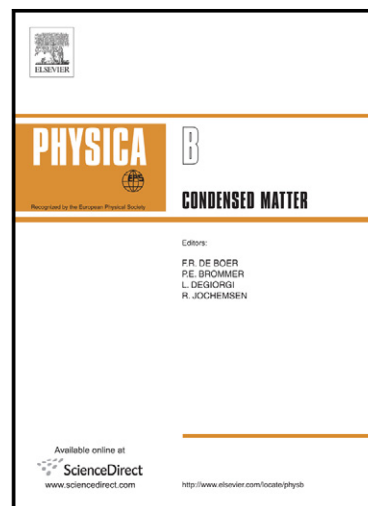


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Svetlana E. Kulkova, Alexander V. Bakulin, Q.M Hu, Rui Yang



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First-principles investigations of oxygen adsorption at TiNi surface and the TiO₂/TiO – TiNi interface

Svetlana E. Kulkova^{1,2,*}, Alexander V. Bakulin¹, Q. M. Hu³ and Rui Yang³

¹Institute of Strength Physics and Material Science SB RAS, pr. Akademichesky 2/4, 634021

Tomsk, Russia

²Tomsk State University, pr. Lenina 36, 634050, Tomsk, Russia

³Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese

Academy of Sciences, Shenyang, China

Abstract. *Ab-initio* 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 TiO₂/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 TiO₂ 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 TiO₂(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 TiO₂. The increase in the formation energies of defects in TiO₂ 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

* Corresponding author at: Institute of Strength Physics and Materials Science SB RAS, pr. Akademichesky 2/4, Tomsk 634021, Russia.
E-mail address: kulkova@ispms.tsc.ru (S.E. Kulkova).

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