ESRF	**Experiment title:** **Reactivity of binary alloys: CO interaction with NiAl(llO)**	**Experiment number:** **SI252**
Beamline: ID3	**Date of experiment:** Feb. 97 from: 20 Februray 1997 to: 27Februray 1997	**Date of report:** **6** March 1998
Shifts: 18	**Local contact(s):** Salvador Ferrer	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

(*)CASTRO, German R.: SpLine-ESRF, Av. des Martyrs, B.P. 220, F-38043 Grenoble
(*)ISERN HERRERA, Helena: ICMM-CSIC, Cantoblanco, E-28049 Madrid
(*)TORRELLES, Xavier: ICMB-CSIC, Campus de la UAB, E-08193
(*)ALVAREZ, Jesus: ESRF, Av. des Martyrs, B.P. 220, F-38043 Grenoble

Report:

The aim of the proposal was to obtain the crystallographic structure of the CO overlayer on NiAl(110). Regard to this objective, the experimental run was unsuccessful, since we were not able to prepare the CO overlayer. However, we have obtained other not less important results related to oxidation of NiAl(110).

Although that for the preparation of the clean surface it was necessary to heat the sample at very high temperatures (- 1200 K) for relatively long time, the vacuum conditions and sample holder were properly. During the CO adsorption and after the preparation of the clean surface, a strong oxygen contamination was observed. Consequently, this surface contamination prevents the formation of the CO (1x4) overlayer. The mean problem has to be related to the users before us, who used very high oxygen dosification for the their sample preparation (adsorption experiments on Rh(111)). Due to the fact that the vacuum chamber had only one pipe for gas inlet, probably the internal pipe wall was oxygen saturated with the consequently gas contamination. The sticking coefficient (S_{CO}) of CO on NiAl(110) is very low (- 10^{-3}), while the S_o for oxygen is 1. Additionally, the binding energy of CO on NiAl(110) is very low (desorption temperature near 273 K), in comparison with the value for oxygen. In the next experiment, we have to be sure that the gas inlet is properly clean.

However, after we release that a strong oxygen contamination (at least for experiments on NiAl(110)) was present, we decided to start with the study of NiAl(110) oxidation. The NiAl(110) clean surface was prepared by several cycles of sputtering and subsequent annealing. The preparation of the ordered Al_2O_3 films was performed as reported in the literature. After a 1200 L O_2 dosification at 500 K and subsequent annealing to 1200 K for few minutes, the well-ordered Al_2O_3 films was formed. Since the oxidation experiment was started relatively late we did not try to resolve the structure of the formed oxide films, rather we try to obtain the structure of the interface between the films and the substrate. Therefore we have measured the (0,l,L); (1,0,L) and (1,l,L) families of non-equivalent NiAl(110) CTR'S from the clean and oxidized surface. From the determined data, structure and composition of the clean surface are in good agreement with the reported ones, i.e, the NiAl(110) surface contains a 1: 1 stoichiometric ratio of Ni and Al atoms with a rippled relaxation. The separation between the Ni and Al top layer is - 0.22 Å with the Al atoms farther from the bulk. The NiAl(110) substrate just below the oxide film persevere the ideal stoichiometry with a similar rippled reconstruction, but the Al atoms in the interface are displaced outwards twice the value corresponding to the clean surface. This results are in preparation for publication.

Due to the fact that the CO experiment could not be realized rather for technical reasons than intrisecal problems of the studied system, I want to ask for a new oportunity to repeat this experiment.