

Oxidation and Modification of NiAl(100)

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Alumina (Al_2O_3) is widely used as a catalyst or a support for various catalysts such as metals and metal oxides. In studies of chemical reactions occurring on these surfaces, a thin film of Al_2O_3 formed by oxidation of NiAl is utilized as a model for the oxide support in catalysts. The thin layer of Al_2O_3 on NiAl has several experimental advantages over bulk oxides involving use of electron spectra to investigate the surface reactions. The Al_2O_3 layer serves as a template for the growth of self-organized metal nanoparticles, and also suppresses the magnetic interaction between those nanoparticles. A considerable effort has thus been devoted to investigate the growth of Al_2O_3 films on a NiAl surface.

The chemical identity of a surface species on the NiAl surface was characterized with XPS and LEED measurements. Upon annealing to 1270 K, the clean NiAl(100) surface exhibits a distinct LEED pattern of two $c(\sqrt{2} \times 3\sqrt{2})R45^\circ$ and $c(3\sqrt{2} \times \sqrt{2})R45^\circ$ domains, as shown in Fig. 1(a).

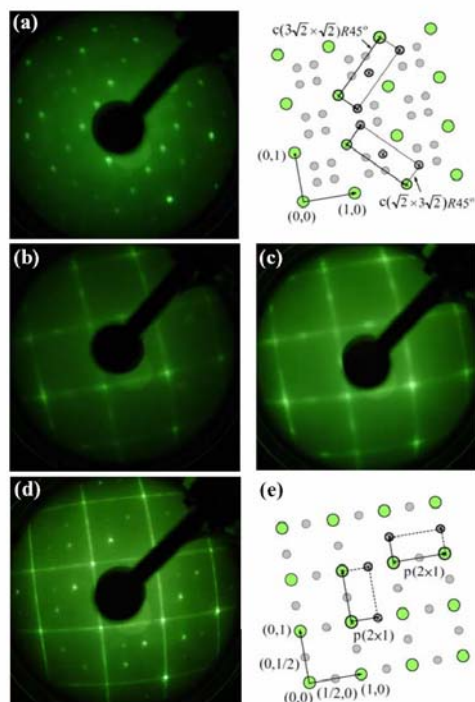


Figure 1. (a) LEED pattern ($E_p = 125$ eV) and schematic representation of clean NiAl (100) with the mixed $c(\sqrt{2} \times 3\sqrt{2})$ and $c(3\sqrt{2} \times \sqrt{2})$ domains. (b)-(d) LEED patterns of NiAl(100) exposed to H_2O at 110 K and annealed to 870 K, 1070 K, and 1270 K, respectively ($E_p = 134$ eV). (e) LEED schematic representation of NiAl(100) with the mixed $p(1 \times 2)$ and $p(2 \times 1)$ domains.

Al_2O_3 thin films are generally prepared on exposing a NiAl surface to an atmosphere of H_2O or O_2 at elevated temperatures. Fig. 2 shows a comparison of Al 2p, Ni 3p, and O 1s spectra of an oxide layer obtained on exposing the NiAl surface to H_2O for 300 s at varied temperatures. In general, the full width at half maximum (FWHM) of the photoelectron peak can serve as indicative of the film quality. The FWHM of the O 1s signal for Al_2O_3 obtained at 970 K (1.8 eV) is slightly smaller than that observed at 870 K (2.0 eV), indicating that the quality is uniform at these temperatures. The intensities of O 1s and Al 2p signals due to Al oxide are smaller for Al_2O_3 grown at temperatures above 1070 K than at 970 K because of the decomposition and evaporation of Al_2O_3 . Similar results were obtained for the growth of Al_2O_3 on exposing the NiAl surface to O_2 , but a greater pressure of oxygen is needed because of its small sticking coefficient.

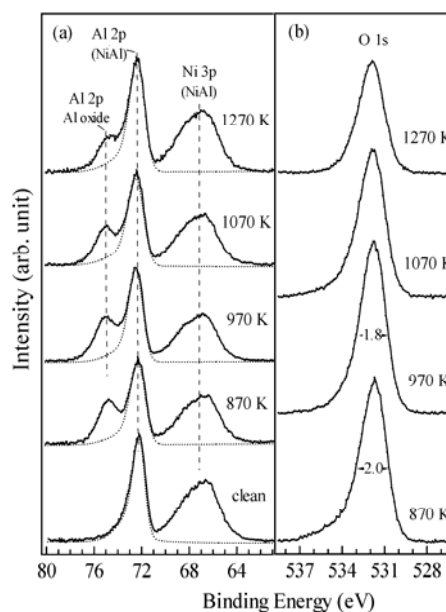


Figure 2. XPS spectra of Al 2p, Ni 3p, and O 1s recorded for the NiAl surfaces exposed to a direct dosing of H_2O for 300 s at 870, 970, 1070, and 1270 K, respectively. The photon energy used to collect the spectra is 650 eV.