morphology. However, both the shape and the orientation differ markedly from those obtained without surfactant. The symmetry axes of the intensity distribution in Figure 3 are rotated 45 degrees compared to those in Figure 2, indicating that the surfactant has caused the pyramid-like islands to grow in a different orientation. The bases of the pyramids are in this case aligned with the [100] surface directions which consist of lines of atoms separated $\sqrt{2}$ times the nearest neighbor atomic spacing. It appears that in some way the surfactant facilitates surface diffusion along the above directions.

The above examples illustrate how two-dimensional images may reveal very important information that would be inaccessible if only one-dimensional intensity profiles were recorded.

Fig. 2: Diffuse scattering distribution after deposition of 27.5 atomic layers. A four-fold symmetry is an evident indicative of ordering.

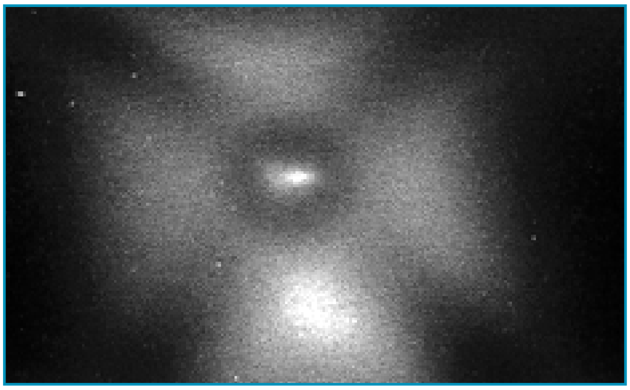
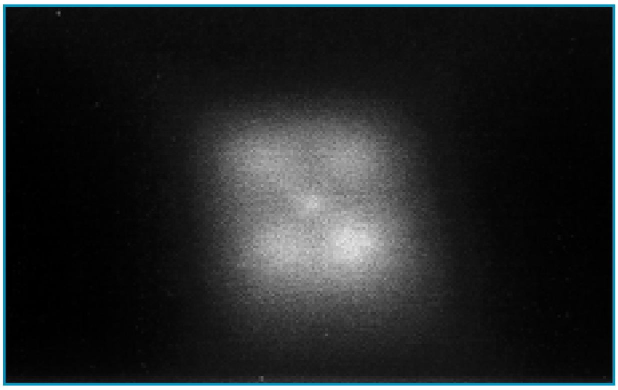


Fig. 3: Diffuse scattering distribution after deposition of 10.5 monolayers of Ag on a Ag(100) surface pre-covered with a small amount of In. The image shows again a four-fold symmetry but the axes are rotated 45° compared to those in Figure 2.



Oxidation of NiAl(100) Studied with Surface Sensitive X-ray Diffraction

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Thin, ordered aluminium oxide layers play a very important role as supports for model catalysts prepared under UHV conditions. Oxidation of NiAl single crystals provides an elegant way to prepare ordered Al_2O_3 layers, which can have different structures depending on the orientation of the NiAl substrate. In addition NiAl is frequently used as a high temperature resistant material. The formation of the protective Al_2O_3 layer is not understood in detail and a microscopic picture of the oxidation process is still missing.

GEED investigations [1] show a (2*1) superstructure after high temperature oxidation and from additional EELS measurements the formation of θ-Al_2O_3 was deduced. The aim of our study was the determination of the Al_2O_3 layer structure and the structure of the Al_2O_3/NiAl(100) interface using surface sensitive x-ray diffraction. The clean sample surface was prepared in the *in situ* UHV surface diffraction chamber of ID32 by several cycles of oxidation and flashing to 1150 °C, which removes the oxide layer and other impurities. Figure 1 shows the structure factor of the clean NiAl(100) surface truncation rods as a function of the reciprocal lattice co-ordinate L normal to the surface.

We tried different models to simulate the data. In model 1 the ideal Ni bulk

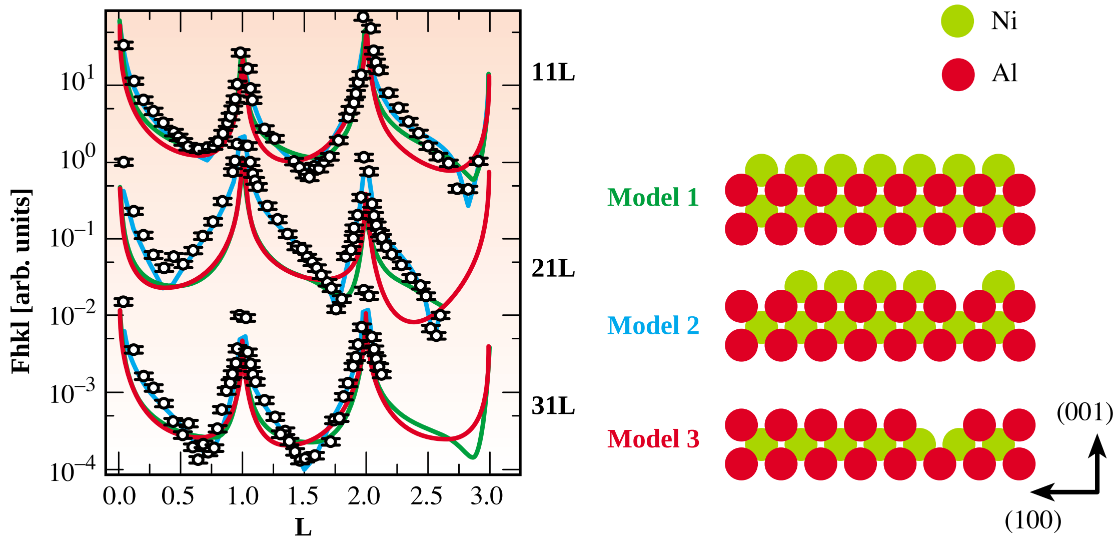

Fig. 1: a) Structure factor F(hkl) as a function of the perpendicular reciprocal lattice co-ordinate L; b) different structural models used to describe the experimental data.

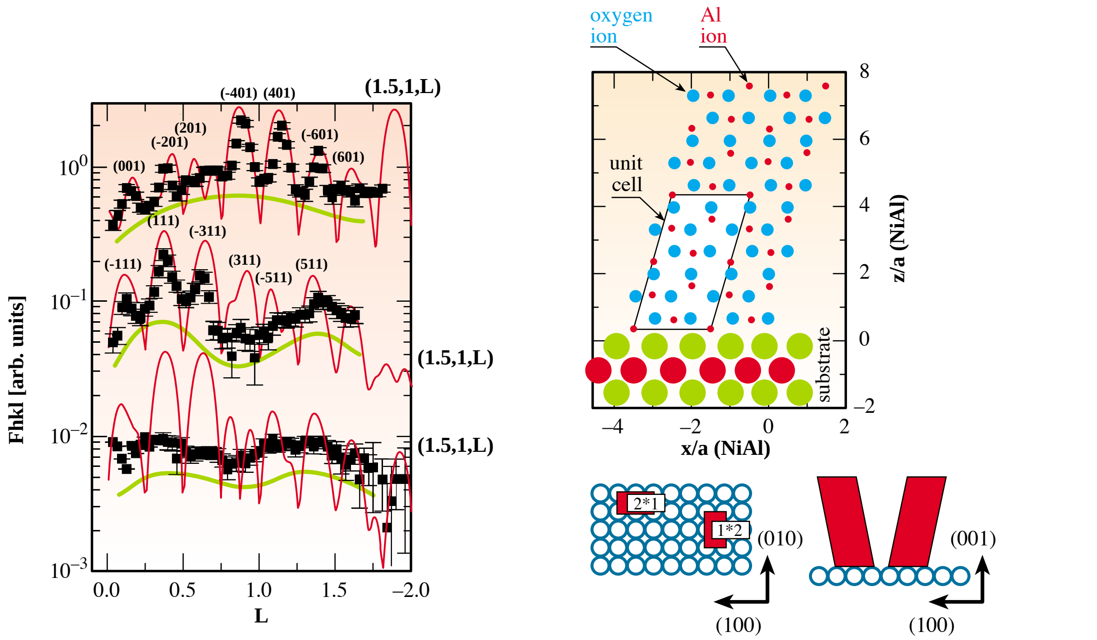

Fig. 2: a) Structure factor F(hkl) of half-order rods after oxidation, b) structural model, c) domain structure.

termination of NiAl with CsCl structure was used and only a relaxation of the first Ni layer was admitted. The simulation could be significantly improved by the introduction of Ni vacancies on the surface (model 2, blue curve) and a 2/3 Ni occupation with 4 % inward relaxation gives the best agreement. An Al terminated surface (model 3), including vacancies and relaxations, is not able to describe the data.

After oxidation at 950 °C for 600 s at $p(O_2)$ = 1 x 10^{-6} mbar half-order rods corresponding to the (2*1) reconstruction appear. In Figure 2 the structure factor as a function of L is plotted for different half-order rods. On all the rods sharper peaks are superimposed on a broad modulation. The red curve is a calculation based on a 2 nm thick monoclinic θ-Al_2O_3 layer; a projection of the structure is shown in Figure 2b. All the peaks observed can be indexed in monoclinic co-ordinates and Figure 2c shows the domain structure of the oxide layer. Besides the (2*1) and (1*2) in-plane domains also twin formation in the growth direction is observed, leading to an inversion of the Al ion layer stacking.

The additional modulation (schematic in green) is attributed to the interfacial structure. At the moment the formation of an Ni_2AlO_4 spinel like interfacial layer is discussed as the origin of the modulation and more detailed model calculations are under its way.

Reference

[1] P. Gassmann, R. Franchy, H. Ibach, Surf. Sci. 319, 95 (1994).