ESRF

Experiment title: Determination of the structure of KCL layers on NaCl

Experiment number: SI-250

Beamline: ID-03

Date of Experiment: from: 18 June 1997 to: 28 June 1997

Date of Report: 29 August 1997

Shifts: 18

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Received at ESRF: 1 SEP. 1997

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Report:

Understanding and controlling the relief of strain during heteroepitaxy is an important scientific and technological goal. Towards that end, we have performed surface x-ray diffraction experiments on the large misfit heteroepitaxial system KCl/NaCl(00l). This system is known from LEED experiments[l] to exhibit two distinct kinds of strain relief behaviors. At 1 ML, the so-called 'floating mode' has been observed[l], where the film retains its natural lattice constant but the height above the substrate is modulated with the period of the misfit repeat distance. However, for films between 2 and 3 ML thick, LEED results show peaks at 75% of the Brillioun zone instead of at expected film Bragg positions. It was was the goal of the present measurement to study and understand the details of this second strain relief mechanism.

The NaCl substrate was prepared by cleaving in air and transferring into the UHV scattering chamber within 15 minutes. The sample was then cleaned by heating to 400 C° for an hour, Rod scans were performed at the specular and at (l,l), (2,0), and (2,2) in order to assess quality of the substrate. Preliminary fitting suggests that the surface is only mildly rough. Data from the clean surface will be analyzed for comparison with models that depend on the evaluation of the long-range coulombic forces in this highly ionic crystal [2].

An example of the layer-by-layer growth achieved in this experiment is pictured in the Figure. This is the intensity of the specular crystal truncation rod at 1=0.53, recorded as a function of time during deposition. The time between the first eight maxima indicate a steady deposition rate of 216 $\pm$ 3 s/ML. In addition to the usual growth oscillations, the intensity has a modulation with a period of 3 ML. This modulation results from interference between layers, and can be reproduced from the simplest possible model: perfect unrelaxed KCL layers on a perfect infinite substrate. KCL and NaCl were given their respective lattice constants, and the KC1 film was placed one KC1 nearest neighbor distance from the substrate.

The effect of the cumulation of defects has been mimicked by subtracting a sloping line. The intensity calculated in this manner is indicated by a dot at each coverage on the figure.

The alkali halide substrates have the advantage in growth experiments that they can be cleaned for a fresh start simply be heating. We could therefore easily study films of several thicknesses in a short time. In this way, films of 1, 2.2, and 2.8 ML thickness were also grown and studied. However, these films showed in each case that the KC1 grows with its own lattice constant. There was very little evidence for superstructure related to the misfit, and no evidence for the different structure seen by Henzler between 2 and 3 ML, despite repeated careful annealings of those films.

In conclusion, this experiment has not fulfilled the goals of studying strain relief at the KCl/NaCl interface. However, we have a data set which may allow the determination of the relaxation of NaCl(001) surface. Furthermore, we have demonstrated that KC1 grows layer-by-layer on NaCl despite the very large misfit.

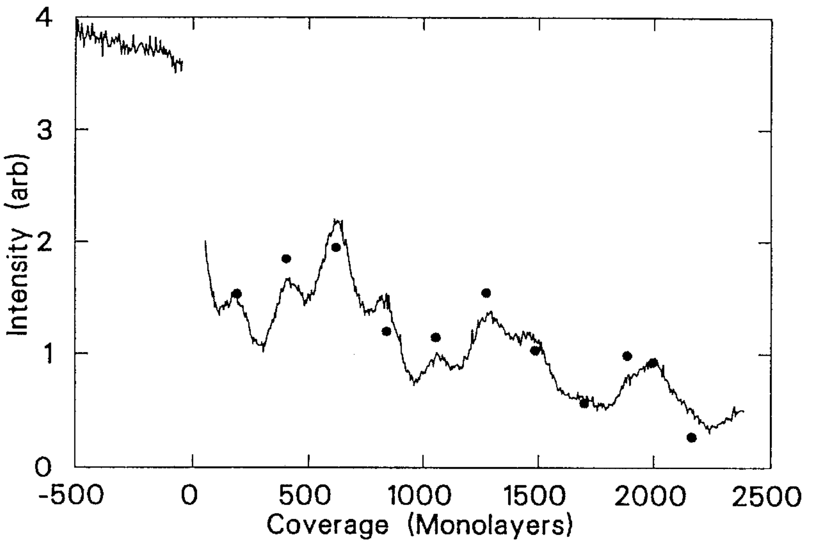

Figure 1: Intensity of the specular rod at l=0.53 vs. time during layer-by-layer growth of KCl/NaCl(001). The dots are from a simple calculation to illustrate that intensity variation is due only to interference between layers.

[l] M. Henzler, C. Homann, and U. Malaske, Phys. Rev. B 52, 17060 (1995)

[2] Jeff Baker and P. A. Lindgard, Phys. Rev. B 54, 11137 (1996)