RHEED (II)

RHEED is used to measure the symmetry and structural parameters of a surface

- Useful in combination with MBE growth
- Can be used up to about $10^{-4}$ Torr
- Is very precise
  - lattice parameter variations of up to one-thousandth of an Angstrom can be seen
  - absolute calibration possible to one-hundredth of an Angstrom

Example Case: manganese nitride

Growth of manganese nitride on magnesium oxide (001)

- several different phases possible
- each phase has specific values of lattice parameter
- various phases have variations of the rock-salt structure

We began growing Mn-N phases in summer 2000 in Smith MBE lab

- First experiments showed very good results by RHEED and STM
- STM images showed a row-like structure
- However, difficulty in deciding what phase/orientation we grew
Manganese nitride growth with RHEED analysis

Careful Analysis reveals several points concerning the data:

First of all, Mn-N RHEED patterns have much similarity to MgO(001) RHEED patterns but with shift of lattice spacing (this is not totally obvious by eye)

\[ a_{\text{MgO}} = 4.213 \text{ Angstrom} \]

\[ a_{\text{Mn}_3\text{N}_2} = ?? \]
To answer the questions, we have to make a careful analysis of the spacing of the streaks.

One can see that the RHEED patterns along both [100] and [110], the pattern for the Mn-N is quite similar to that of the MgO except for:

- along [100], Mn-N pattern shows fractional (1/3rd) order streaks
- along [100], Mn-N pattern shows split integral (1st) order streaks

To analyze the data, we need precise values for the lattice spacings for the Mn-N mathematically:

\[
\text{streak spacing } S \sim [\text{lattice constant, } a]^{-1}
\]

or

\[
S \sim 1/a
\]

So,

\[
S_{\text{MgO}} \sim 1/a_{\text{MgO}}
\]

\[
S_{\text{Mn-N}} \sim 1/a_{\text{Mn-N}}
\]

Therefore, if \(a_{\text{MgO}}\) is known,

\[
a_{\text{Mn-N}} : a_{\text{MgO}} = S_{\text{MgO}} : S_{\text{Mn-N}}
\]

In this way, one can solve for \(a_{\text{Mn-N}}\)

Important Complication: if the two RHEED patterns were acquired at different temperatures, then thermal contraction has to be taken into account.
So, let’s look in detail at the line sections of the RHEED patterns for MgO and Mn-N

Looking carefully, we see:

- one-3\textsuperscript{rd} order streaks coincide with outer integral streak
- split-integral order streaks superimposed on each other
  - need to separate them carefully from each other

To get the accurate value of lattice constants for Mn-N, had to correct for thermal contraction since MnO pattern was at 450°C whereas Mn-N pattern was at 25°C
In practice, we can say that if the MgO RHEED had been acquired at 25°C, then the lattice constant would have been smaller and the streak spacing $S$ would have been larger.

Therefore, we measure the MgO streak spacing $S$ and multiply by a number equal to $1.1 > 1$ to get $S_{\text{MgO}}(25^\circ\text{C})$.

given $S_{\text{MgO}}(25^\circ\text{C})$, we focus on the Mn-N streak spacings.

To the Mn-N streaks spacings $S_1$ and $S_2$, it is necessary to do a peak fitting method, or to use peak fitting software.

We did this at the time “by hand” using Lorentzian peak fitting as follows:

First, we extract the line profile data and plot it carefully.

Then we use two Lorentzian functions added together to model the total split-peak line profile:

$$L(x) = \frac{A_0}{4\left(\frac{(x - x_0)}{\sigma}\right)^2 + 1}$$

$A_0$ = amplitude of Lorentzian

$x$ = position $x$

$x_0$ = centroid

$\sigma$ = width of Lorentzian
Lorentzian Fitting results for Mn-N data:

After correction for the peak overlap, the split-peaks were found to have a difference in spacing

\[
\frac{(S1 - S2)}{S_{ave}} = 4\%
\]

In particular,

lattice spacing \( s_1 = 2.103 +/- 0.002 \) Å

lattice spacing \( s_2 = 2.023 +/- 0.002 \) Å
We then went on to identify that:

\[ s_1 \text{ corresponds to } a_{\text{Mn}_3\text{N}_2}/2 = (4.207 \pm 0.004 \text{ Å})/2 \]

\[ s_2 \text{ corresponds to } c_{\text{Mn}_3\text{N}_2}/6 = (12.141 \pm 0.012 \text{ Å})/6 \]

Both of these lattice parameters were found to occur in the surface plane.

Finally, combining with STM data and a model published earlier from bulk methods, by another group (G. Kreiner and H. Jacobs, J. Alloys Compd. 183, 345 (1992)),

We deduced the structure of the film and the surface of the film: