

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

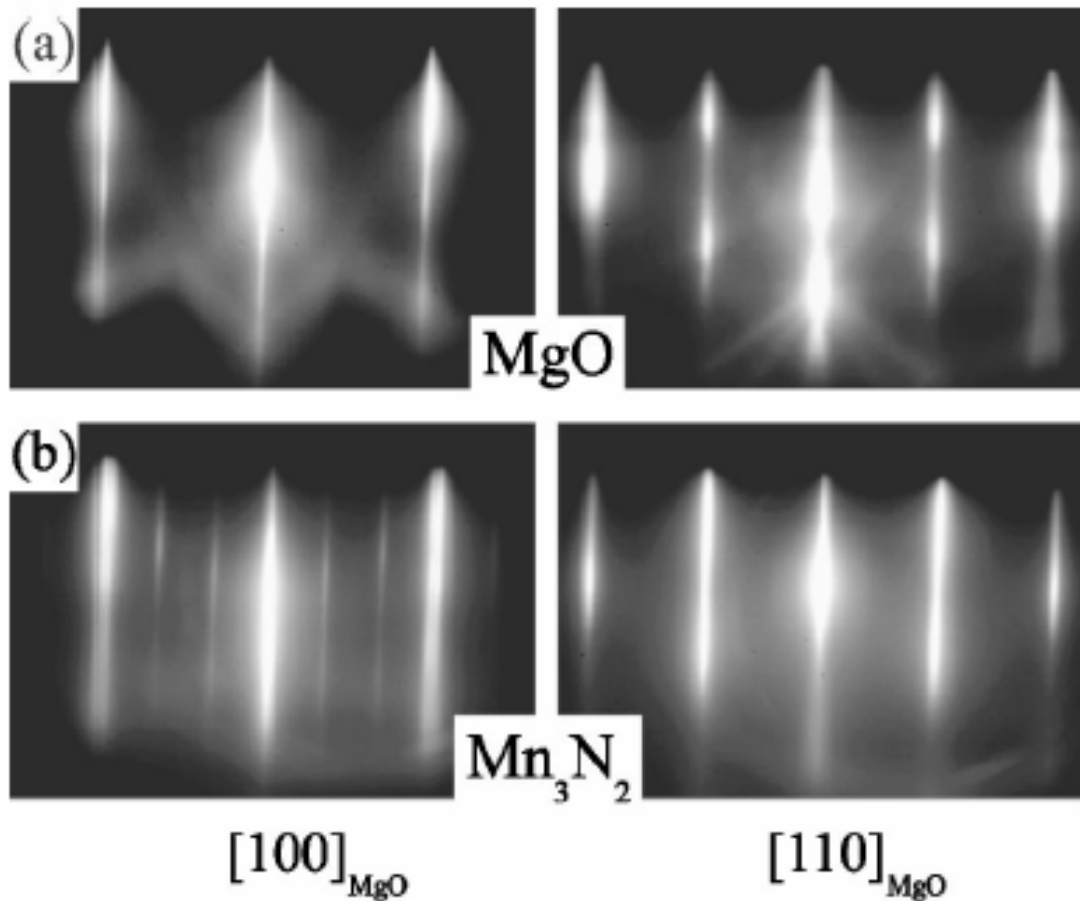
Growth of manganese nitride on magnesium oxide (001)

- 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



- from Haiqiang Yang, Hamad Al-Britthen, Arthur R. Smith, J.A. Borchers, R.L. Cappelletti, and M.D. Vaudin, *Appl. Phys. Lett.* **78**, 3860 (2001).

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)

$a_{\text{MgO}} = 4.213$ 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 ($1/3^{\text{rd}}$) order streaks
- along [100], Mn-N pattern shows split integral (1^{st}) 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_{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

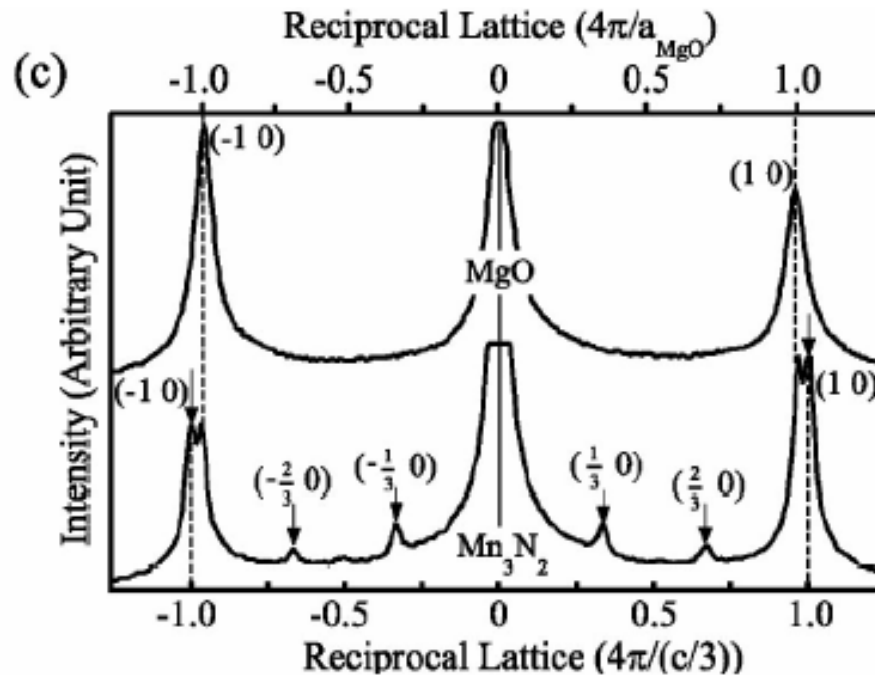


FIG. 1. RHEED patterns and line profiles of MgO and η Mn_3N_2 are shown. (a) MgO surface after 30 min of heating at 1000 °C and cooling down to 450 °C; (b) η Mn_3N_2 surface obtained following growth near 25 °C, left-hand side panel along $[100]_{\text{MgO}}$ and right panel along $[110]_{\text{MgO}}$. (c) Line profiles of MgO (top) and η Mn_3N_2 (bottom) along $[100]_{\text{MgO}}$.

- from Haiqiang Yang, Hamad Al-Brithen, Arthur R. Smith, J.A. Borchers, R.L. Cappelletti, and M.D. Vaudin, *Appl. Phys. Lett.* **78**, 3860 (2001).

Looking carefully, we see:

- one-3rd 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 $1.x > 1$ 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 the Mn-N streaks spacings S1 and S2, 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:

$$L(x) = A_0 / [4((x - x_0)/\sigma)^2 + 1]$$

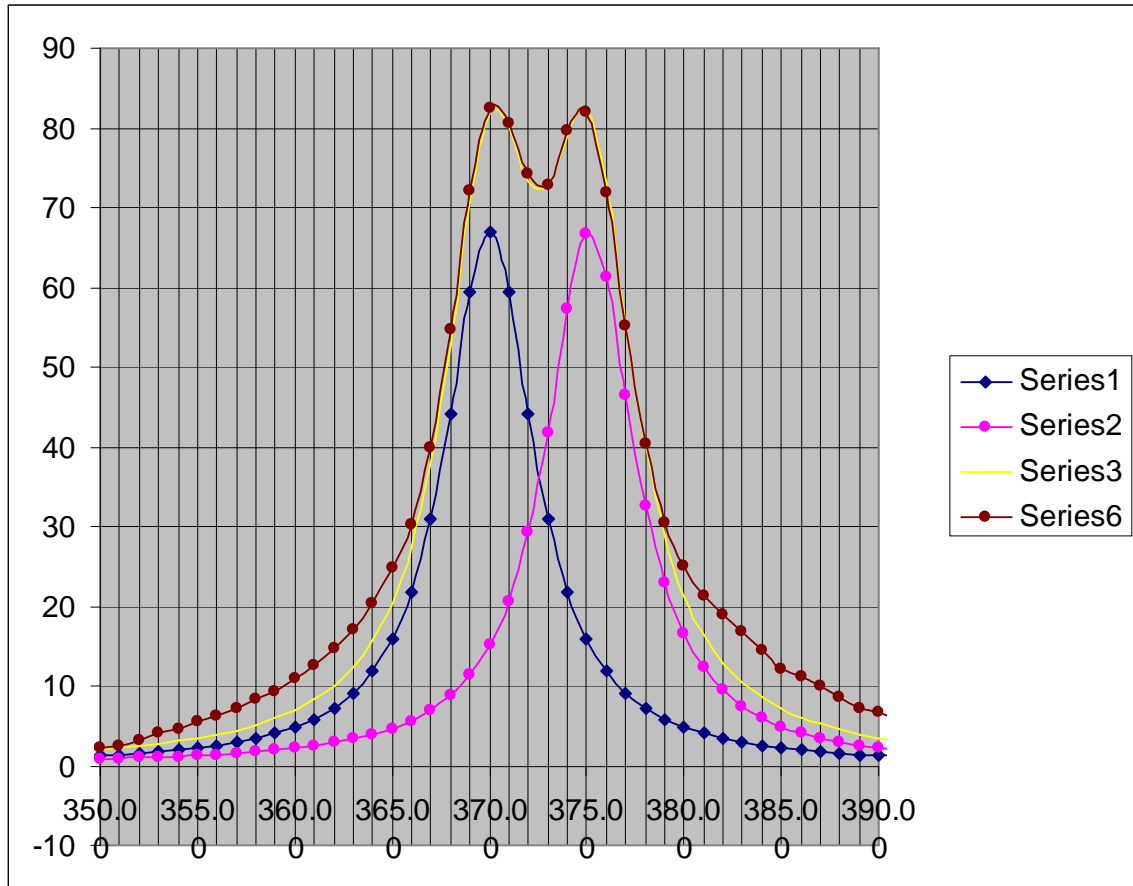
A_0 = amplitude of Lorentzian

x = position x

x_0 = centroid

σ = width of Lorentian

Lorentzian Fitting results for Mn-N data:



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

$$(S1 - S2)/S_{ave} = 4\%$$

In particular,

$$\text{lattice spacing } s_1 = 2.103 \pm 0.002 \text{ \AA}$$

$$\text{lattice spacing } s_2 = 2.023 \pm 0.002 \text{ \AA}$$

We then went on to identify that:

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

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

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:

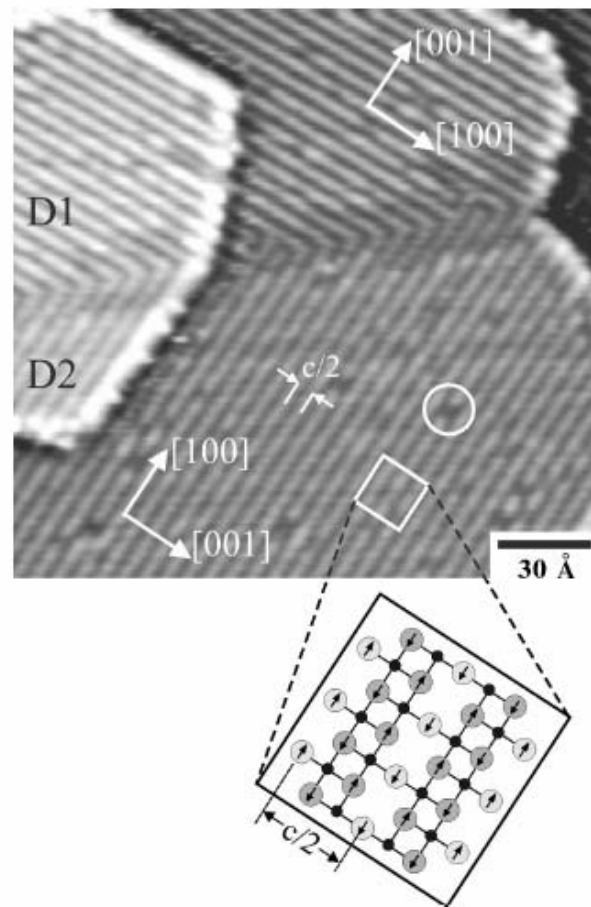


FIG. 4. STM image of η Mn_3N_2 is shown. The image was acquired at a sample bias of -0.4 V and a tunneling current of 0.8 nA. The enhancement at the step edge is due to a local background subtraction. D1 and D2 label two equivalent domains rotated 90° to each other. The white circle marks a point defect. A zoom out shows the corresponding bulk-like model with atoms marked as in Fig. 2.

- from Haiqiang Yang, Hamad Al-Brithen, Arthur R. Smith, J.A. Borchers, R.L. Cappelletti, and M.D. Vaudin, *Appl. Phys. Lett.* **78**, 3860 (2001).