Growth Kinetics of GaN grown by Molecular Beam Epitaxy using Ga and Ammonia

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by

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Bulk GaN Crystals

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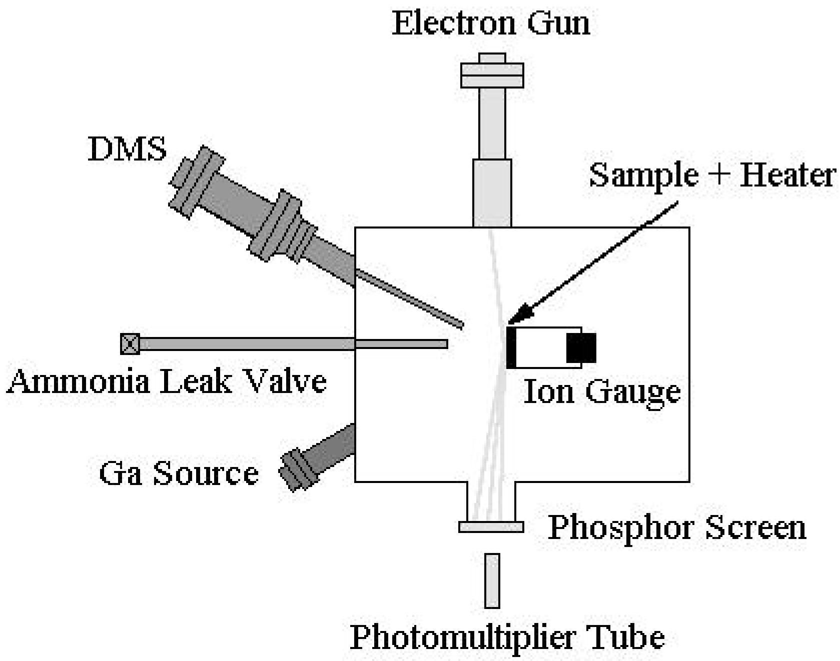
Motivation

- GaN is wide bandgap semiconductor: blue LED, blue Laser, UV detector
- MBE offers better (*in situ*) control over growth than MOCVD
- very little was known about growth mechanism

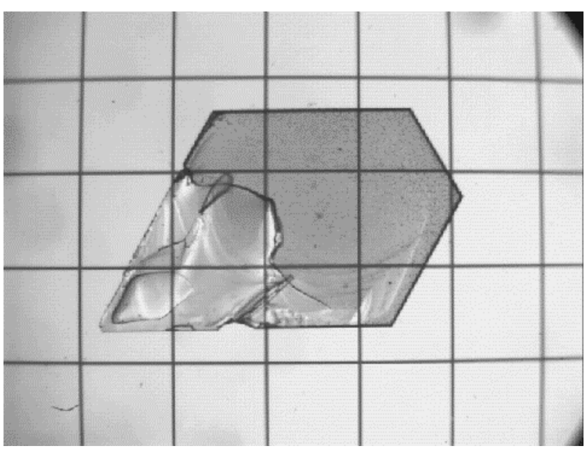
Preview

- instrumentation
- background
- develop model for surface reactivity
- develop model for growth
- surface morphology
- conclusions

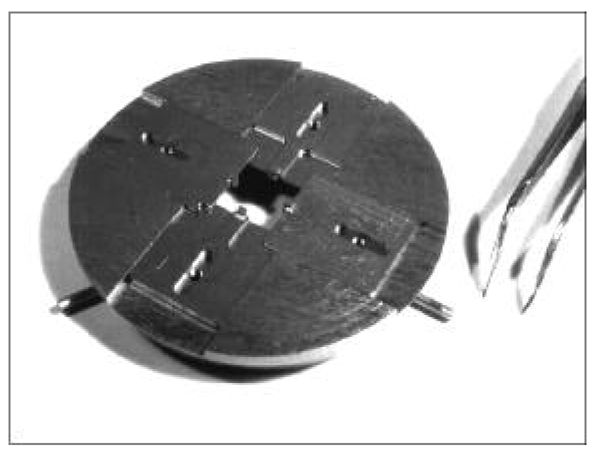
Molecular Beam Epitaxy (MBE)



Samples and Mounting

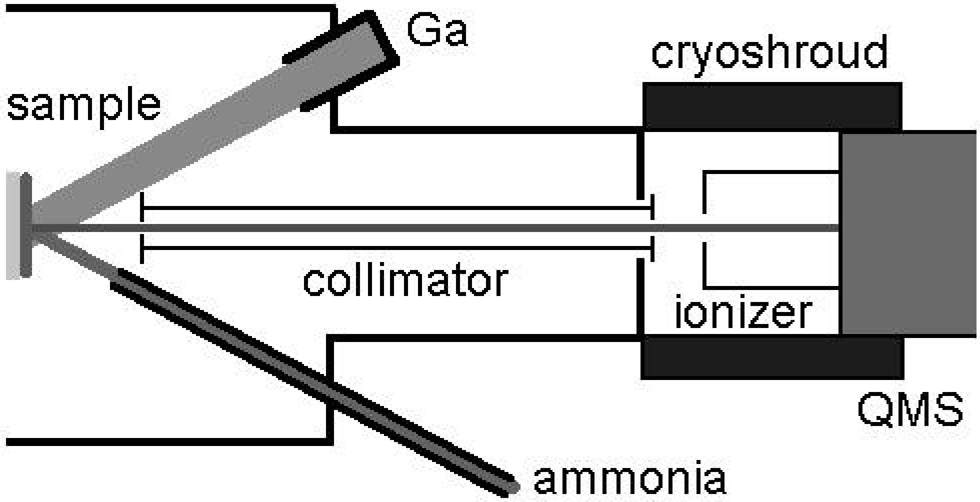


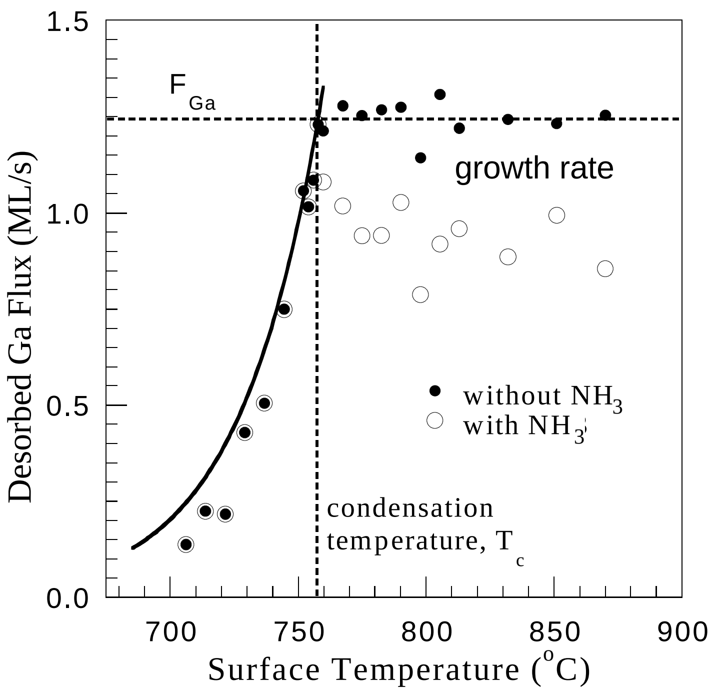
1 mm grid



2 1/4 inch diameter

Desorption Mass Spectroscopy (DMS)





- F_{Ga} from GaAs RHEED intensity oscillations
- T_s from Ga condensation, T_c *

* R. Held, D.E. Crawford, A.M. Johnston, A.M. Dabiran, and P.I. Cohen, *Journal of Electronic Materials*, **26**, 272 (1997)

Background

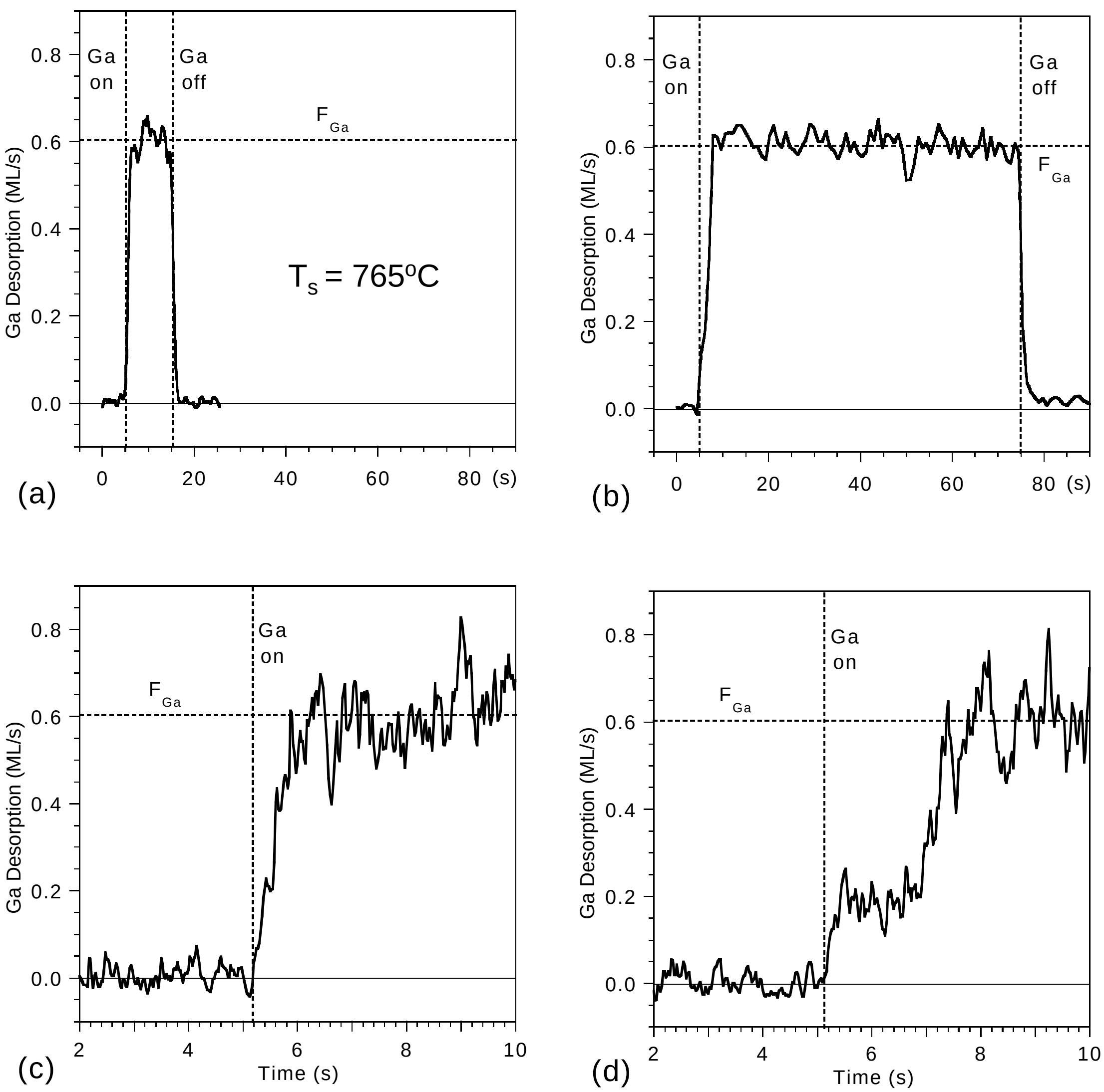
- GaN{0001} is polar
- bulk GaN has both polarities
- polarities can be distinguished [+] [*]
- GaN on sapphire either polarity [*]
- focus on GaN(000$\underline{1}$) or GaN-B
- RHEED showed two possible surface terminations on GaN-B, after Ga or NH_3 only exposure [#]

[+] A.R. Smith, R.M. Feenstra, D.W. Greve, M.-S. Shin, M. Skowronski, J. Neugebauer, J.E. Northrup, *Appl. Phys. Lett.*, **72**, 2114 (1998)

[*] R. Held, G. Nowak, B.E. Ishaug, S.M. Seutter, A. Parkhomovsky, A.M. Dabiran, P.I. Cohen, I. Grzegory, and S. Porowski, *J. Appl. Phys.*, in press

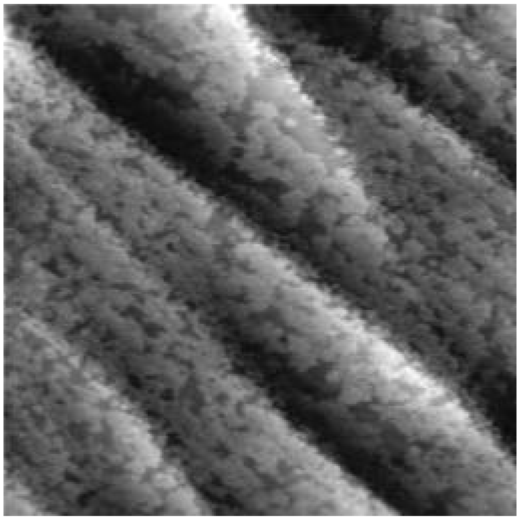
[#] R. Held, D.E. Crawford, A.M. Johnston, A.M. Dabiran, and P.I. Cohen, *Surf. Rev. Lett.*, **5**, 913 (1998)

Surface Reactivity
gallided / nitrided

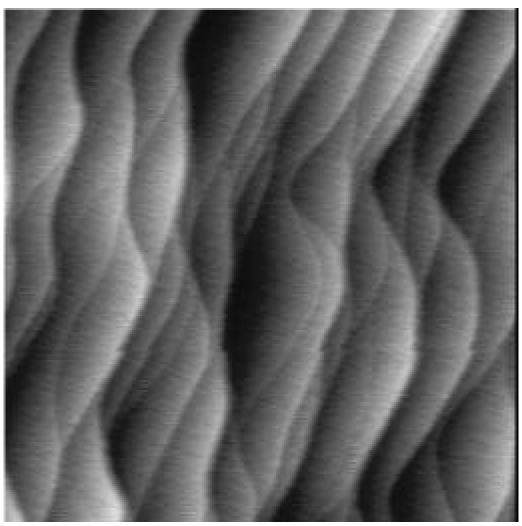


- nitrided surface becomes gallided after Ga exposure
- approx. 0.5-1.0 ML of Ga adsorb strongly
- Ga adsorbs weakly on gallided (q_w)

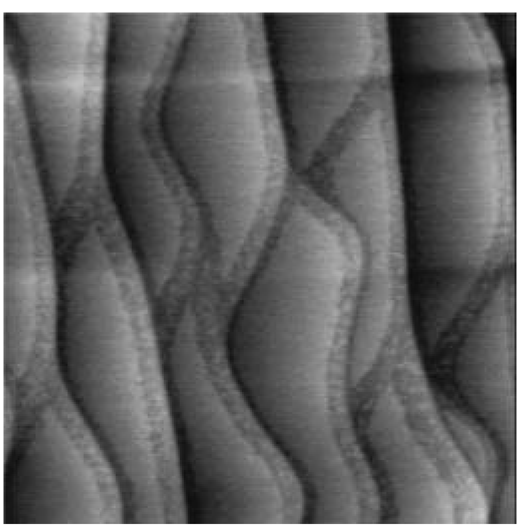
AFM Surface Morphology



nitrided surface $q_s = q_{s,o}$



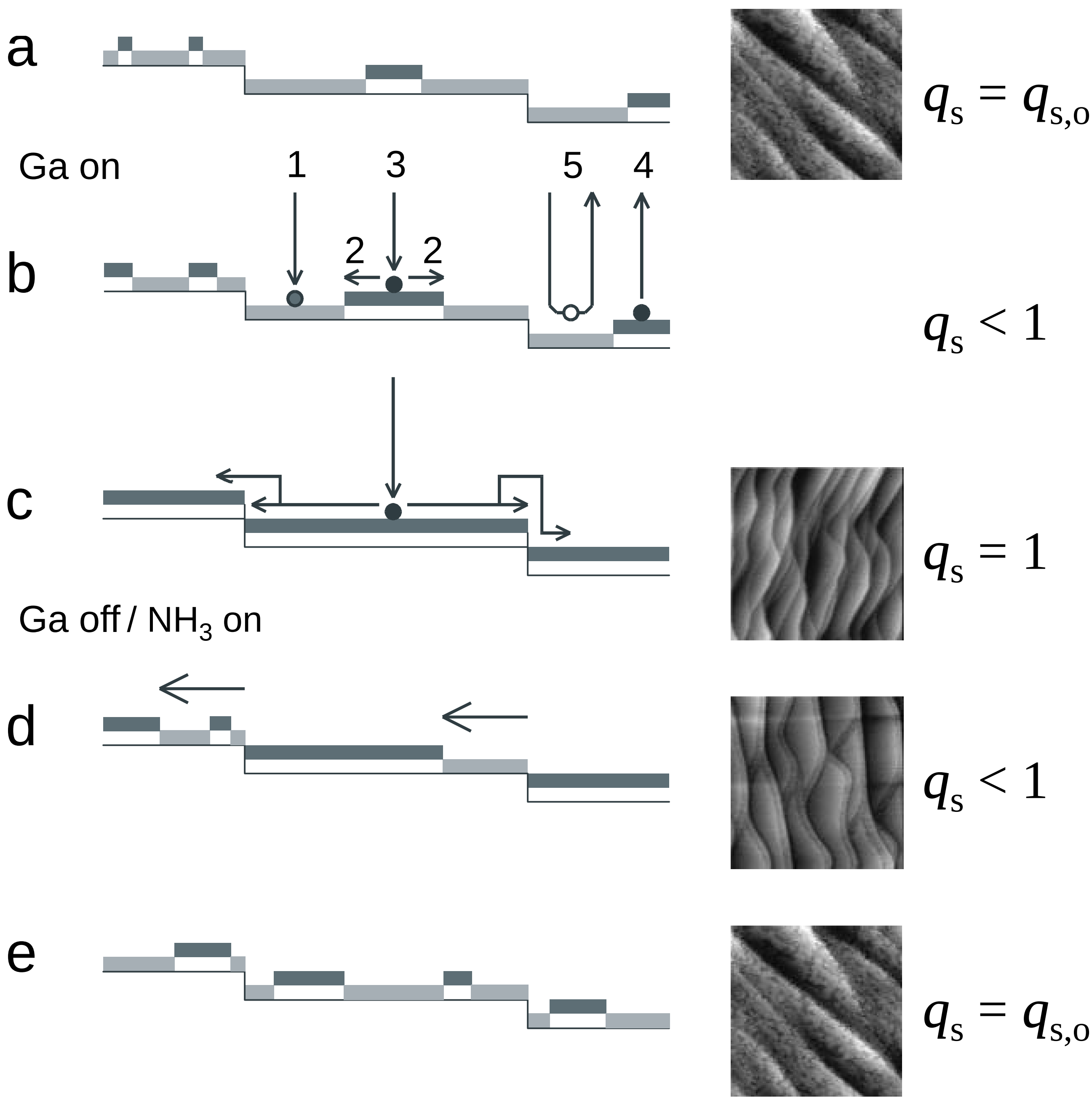
gallided surface $q_s = 1$



anneal gallided in NH_3

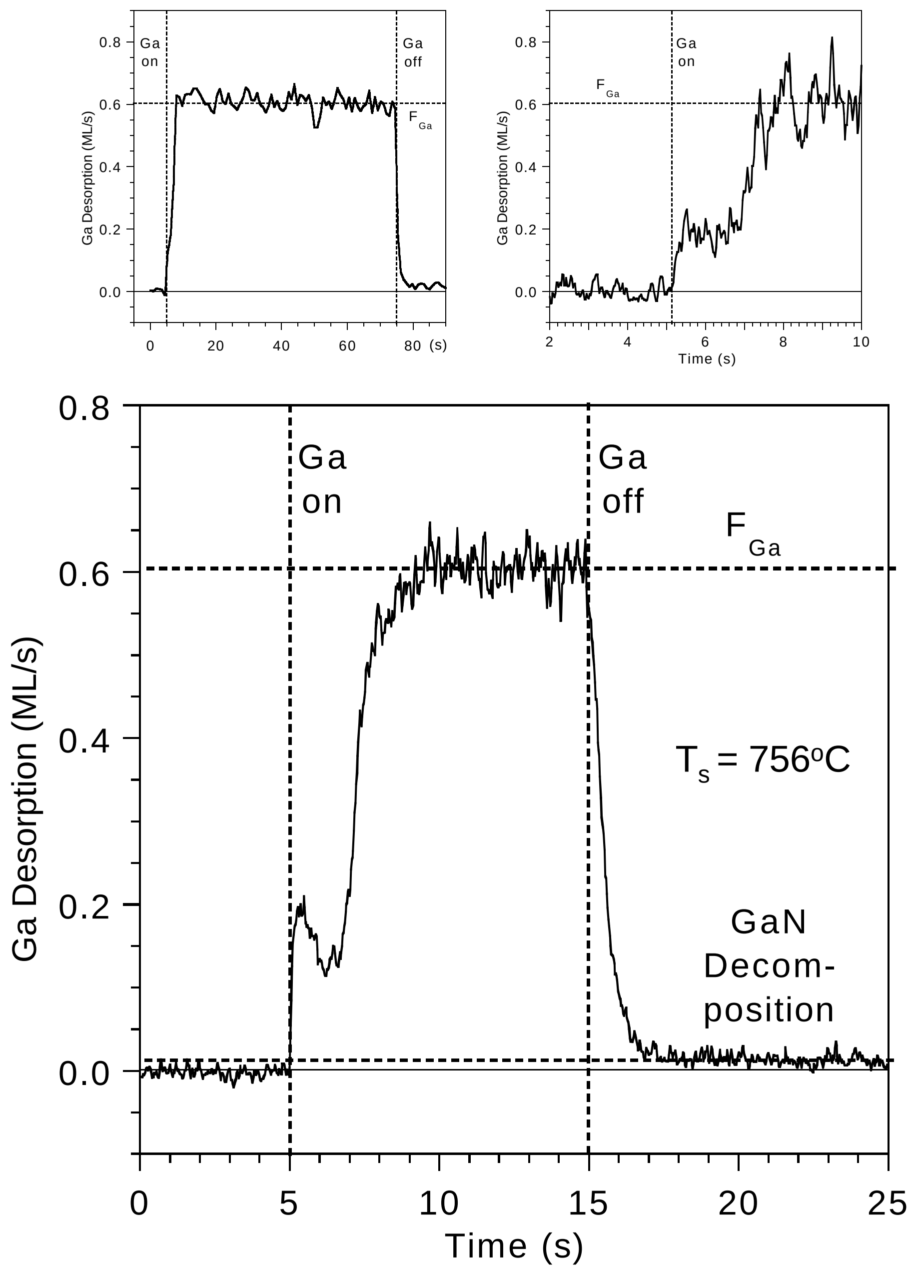
1 μm scans

Basic Model Assumptions



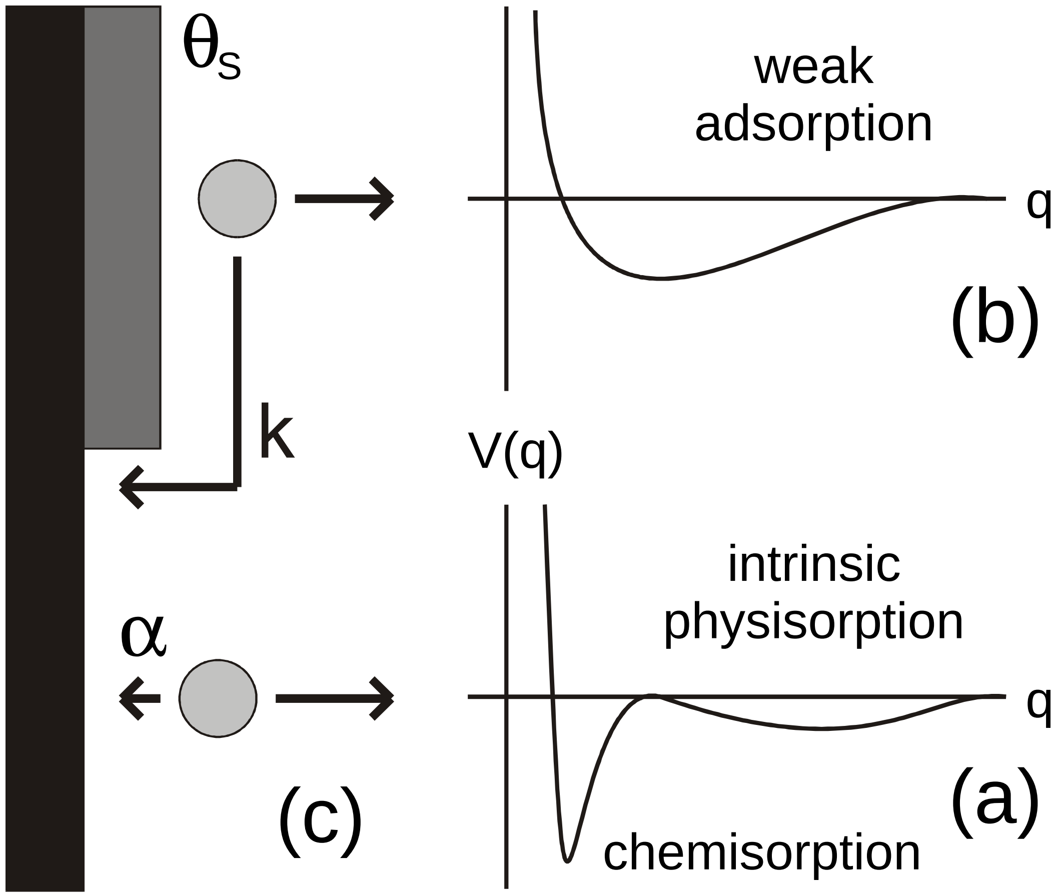
first goal:
develop quantitative model without NH_3

Fast Weak State



- near instantaneous rise suggests fast weak state
- drop in "knee" suggests states proportional to q_s
- drop < > 0 suggests desorption overlaps with q_w

“galliding” Model

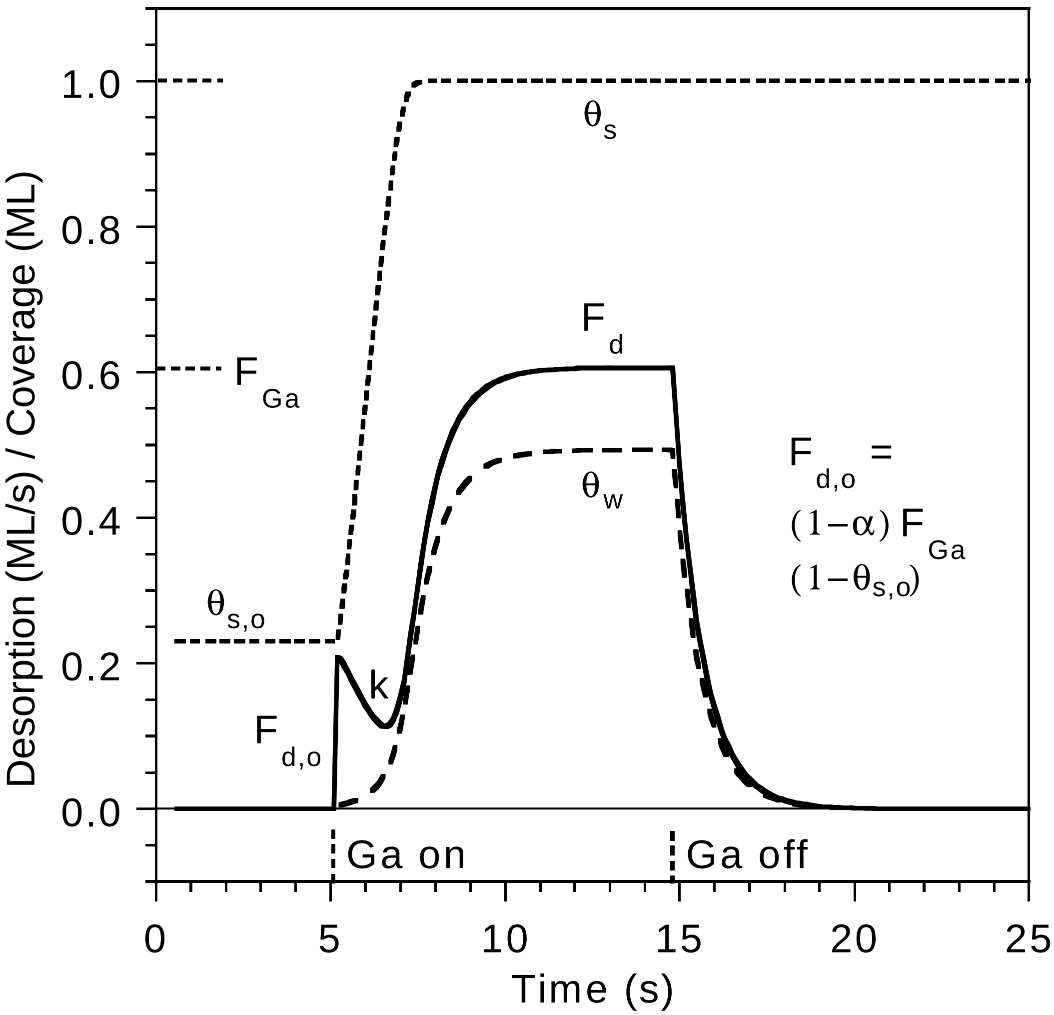


$$\frac{\mathrm{d}q_{\mathrm{s}}}{\mathrm{d}t} = (1-q_{\mathrm{s}})a\ F_{\mathrm{Ga}} + q_{\mathrm{w}}(1-q_{\mathrm{s}})k$$

$$\frac{\mathrm{d}q_{\mathrm{w}}}{\mathrm{d}t} = q_{\mathrm{s}}F_{\mathrm{Ga}} - q_{\mathrm{w}}/t - q_{\mathrm{w}}(1-q_{\mathrm{s}})k$$

$$F_{\mathrm{d}} = (1-a)F_{\mathrm{Ga}}(1-q_{\mathrm{s}}) + q_{\mathrm{w}}/t$$

Fitting Procedure

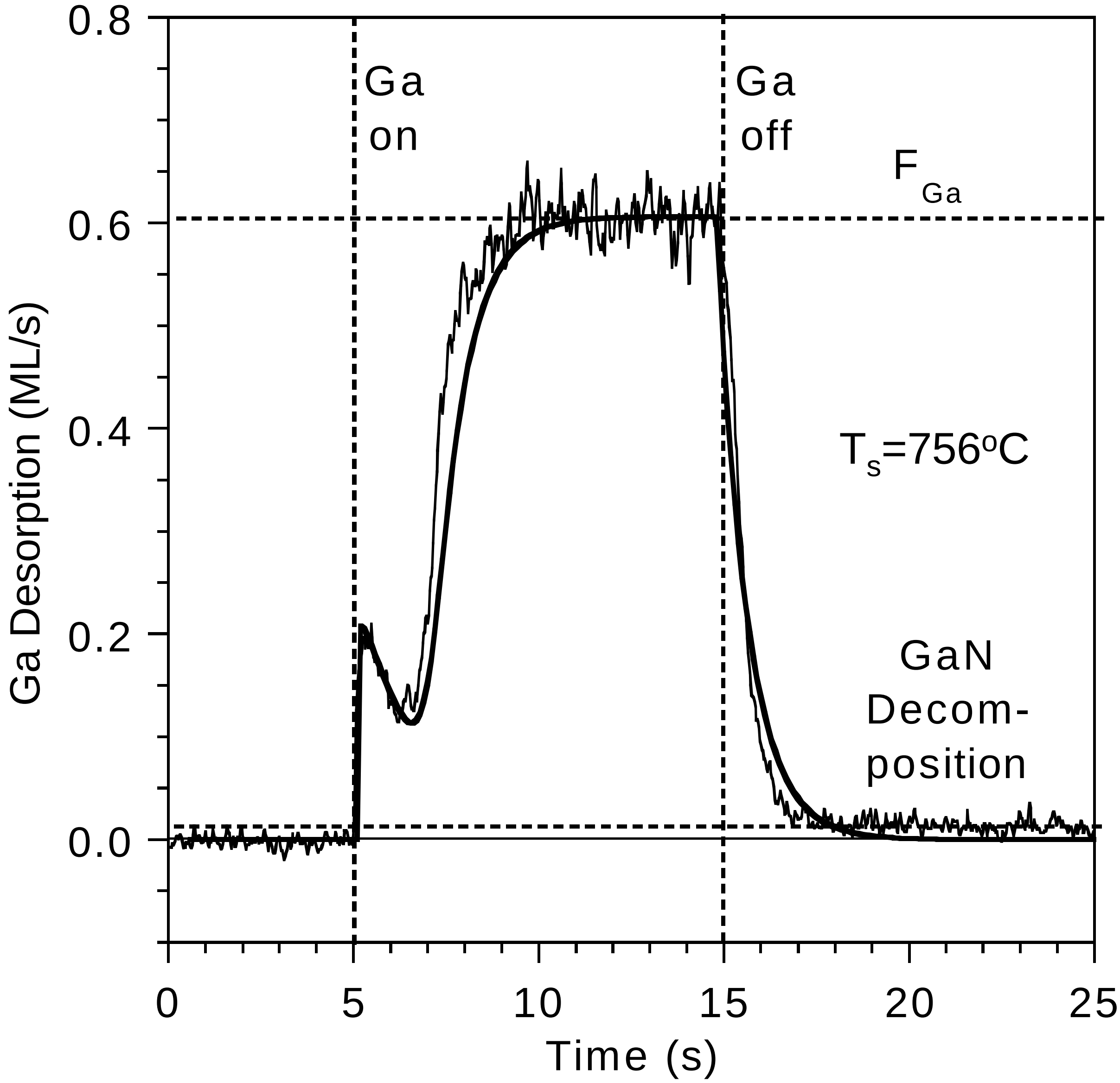


$$\frac{\mathrm{d}q_\mathrm{s}}{\mathrm{d}t} = (1-q_\mathrm{s})a\ F_\mathrm{Ga} + q_\mathrm{w}(1-q_\mathrm{s})k$$

$$\frac{\mathrm{d}q_\mathrm{w}}{\mathrm{d}t} = q_\mathrm{s}F_\mathrm{Ga} - q_\mathrm{w}/t - q_\mathrm{w}(1-q_\mathrm{s})k$$

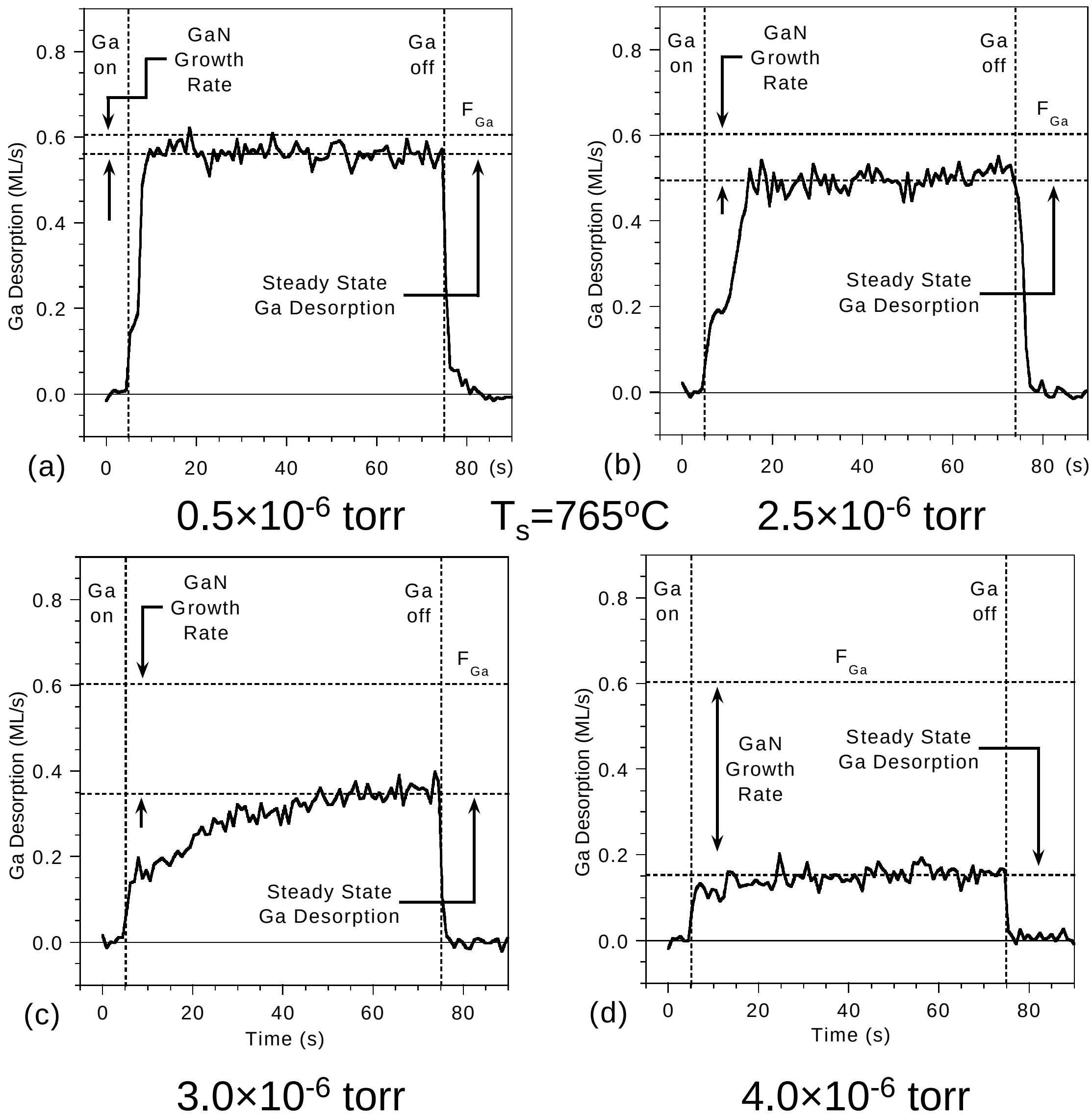
$$F_\mathrm{d} = (1-a)F_\mathrm{Ga}(1-q_\mathrm{s}) + q_\mathrm{w}/t$$

Curve Fitting



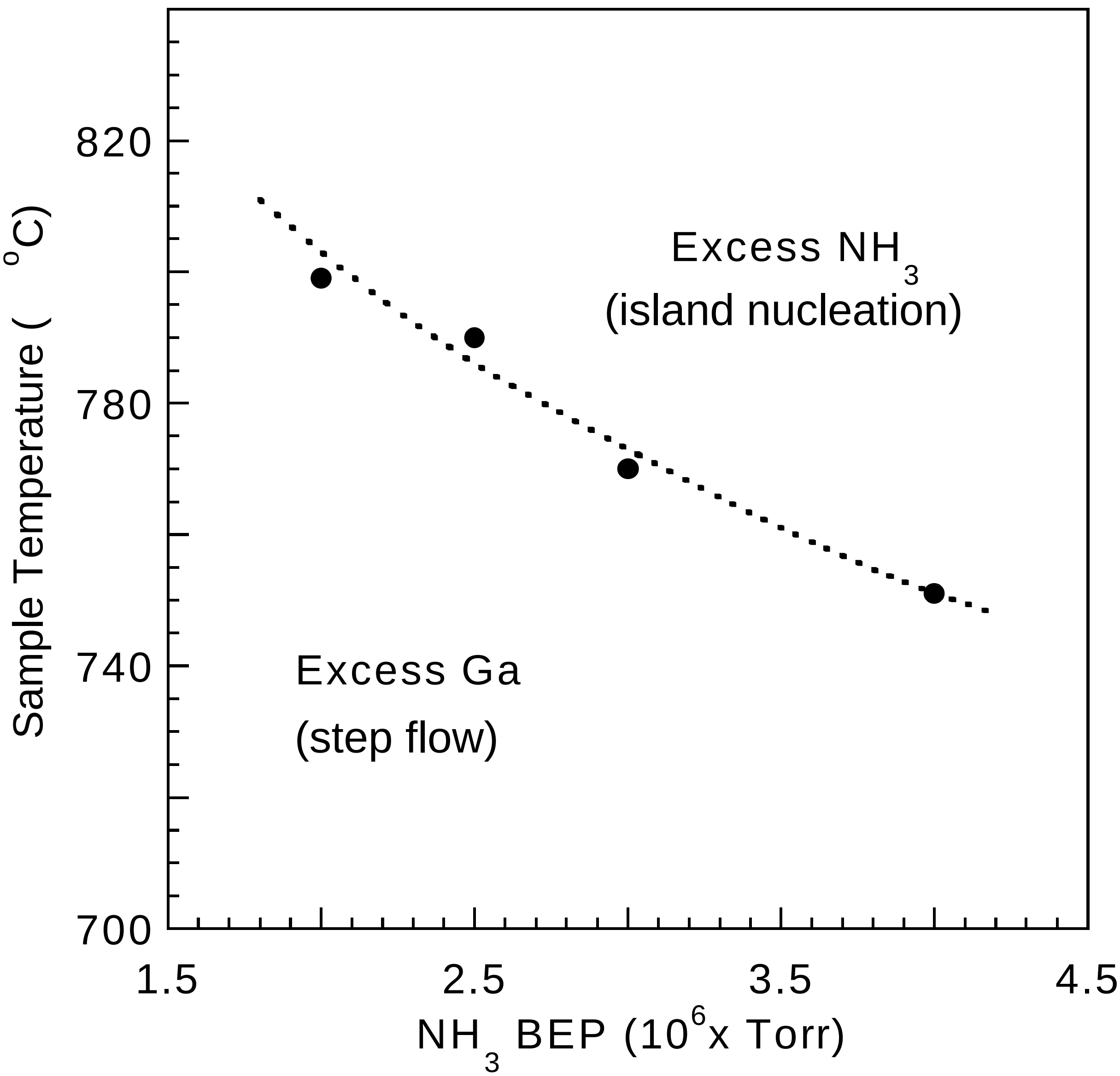
Sample:	**Results:**
$q_{s,o}$ = 0.23 ML	$q_{s,o}$ = 2.62 - 0.00235 T (ML)
a = 0.45	a = 0.5
k = 35 ML/s	$k = 1.2\times10^{7}\ e^{-1.2\ (eV)/kT}$ (ML/s)

Uptake Curves with NH_3



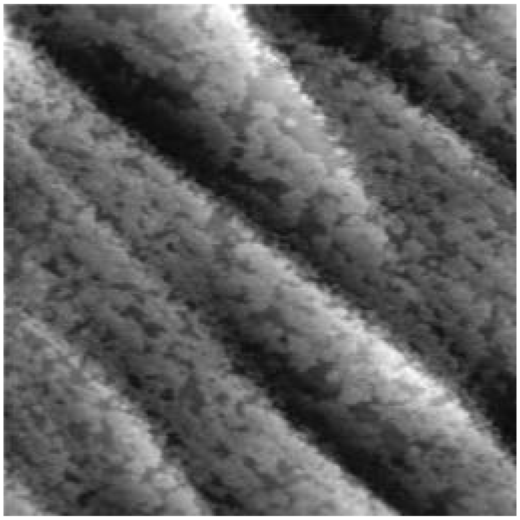
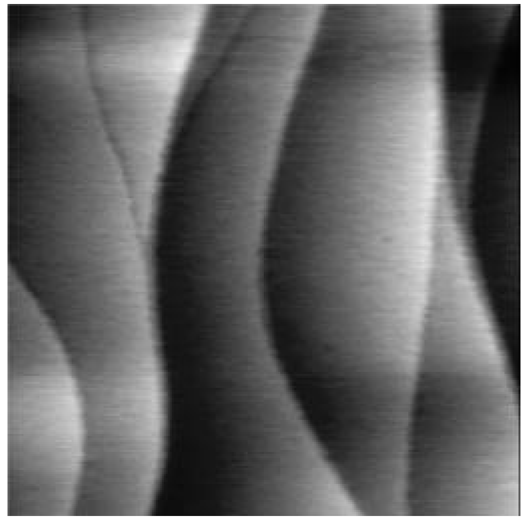
- $F_{Ga} >> F_{NH3}$ like gallided surface, unreactive
- $F_{NH3} >> F_{Ga}$ like nitrided surface, reactive
- abrupt growth regime crossover from
  step flow to island nucleation (AFM, RHEED)

Abrupt Crossover



- would like to expand model to include growth
- model has to feature an abrupt crossover

Growth Terms

excess NH_3 — 1 μm scans — excess Ga

$$\frac{\mathrm{d}q_{\mathrm{s}}}{\mathrm{d}t} = (1-q_{\mathrm{s}})a\ F_{\mathrm{Ga}} + q_{\mathrm{w}}(1-q_{\mathrm{s}})k$$

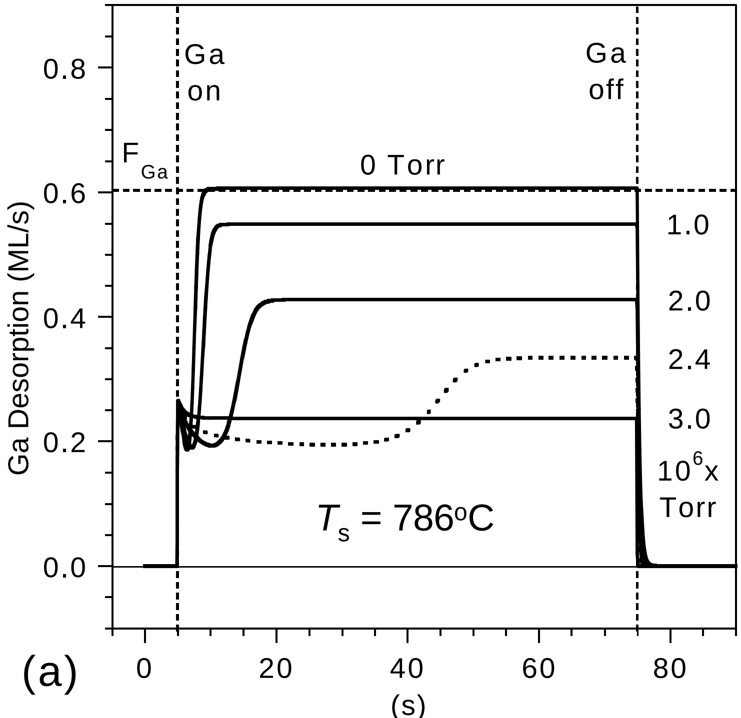
excess NH_3: $$-(q_{\mathrm{s}} - q_{\mathrm{s,o}})^{x}(1-q_{\mathrm{s}})^{x} F_{\mathrm{N}}$$

excess Ga: $$-f(1-q_{\mathrm{w}})(q_{\mathrm{s}} - q_{\mathrm{s,o}})F_{\mathrm{N}}$$

- in both limits one or other term goes to zero
- excess NH_3: island perimeter growth (x = 1/2)
- excess Ga: step edge growth with efficiency parameter f and inhibitation * term

* D.E. Crawford, R. Held, A.M. Johnston, A.M. Dabiran, P.I. Cohen, *MRS Internet Journal NSR*, **1**, 12 (1996)

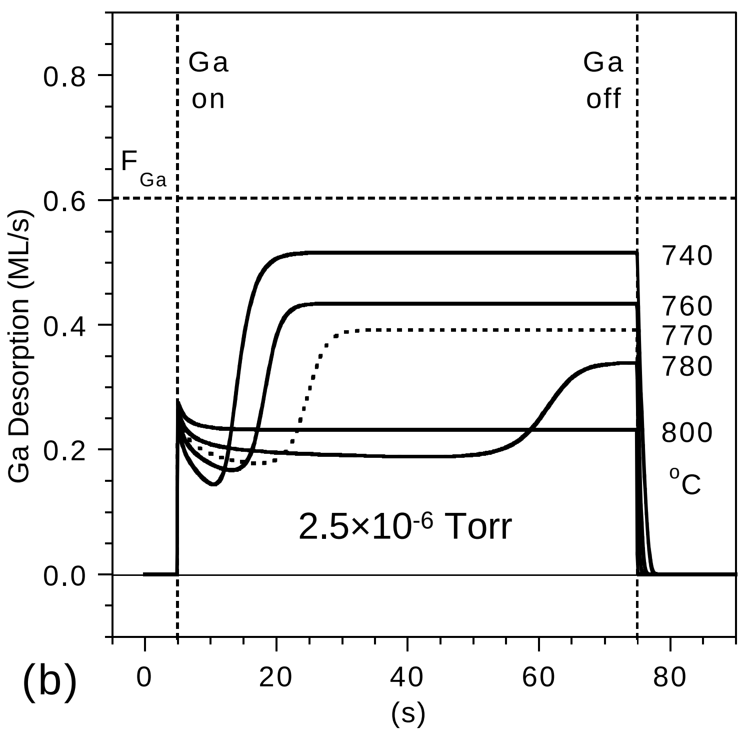
Crossover Modeling



(a)

abrupt crossover versus ammonia

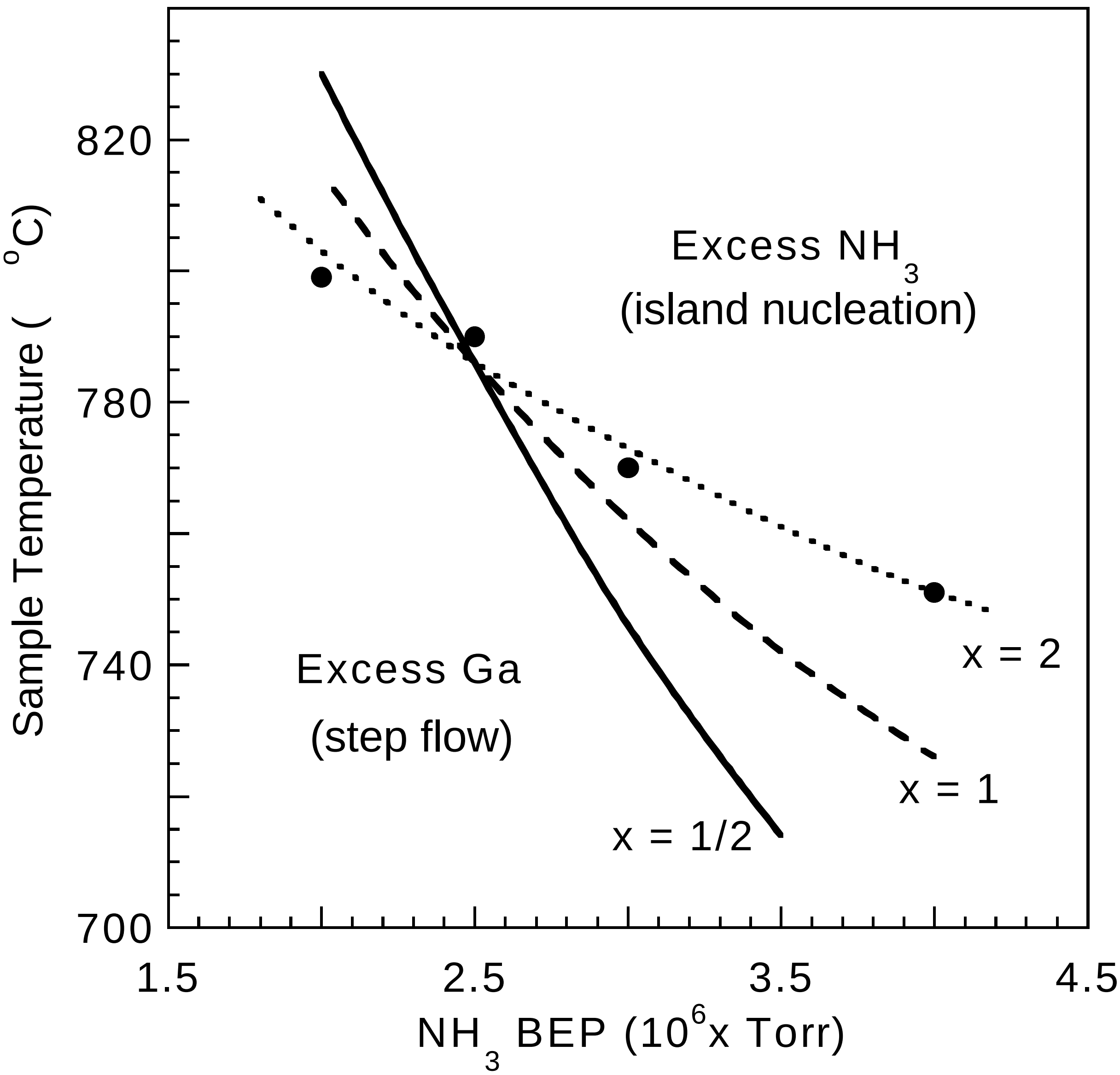
x=1/2



(b)

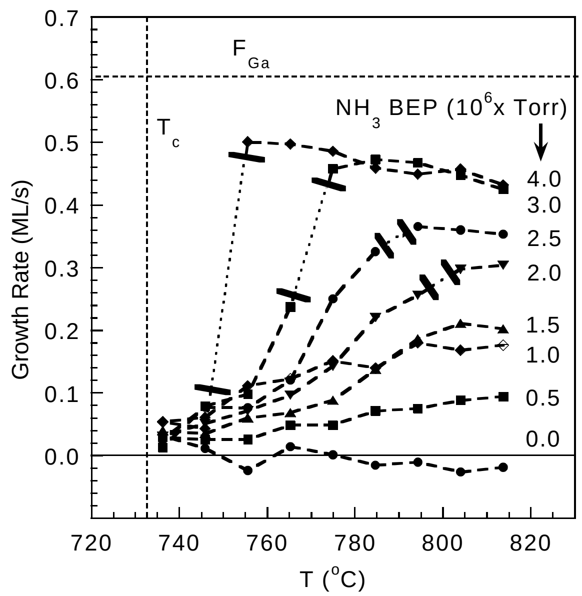
abrupt crossover versus temperature

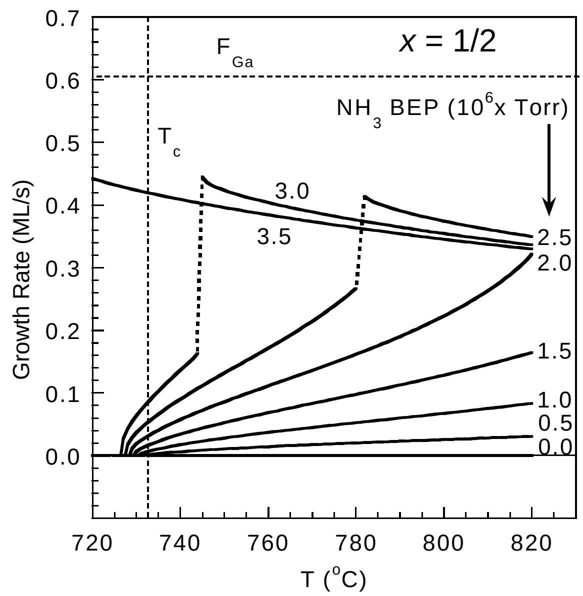
Crossover Results

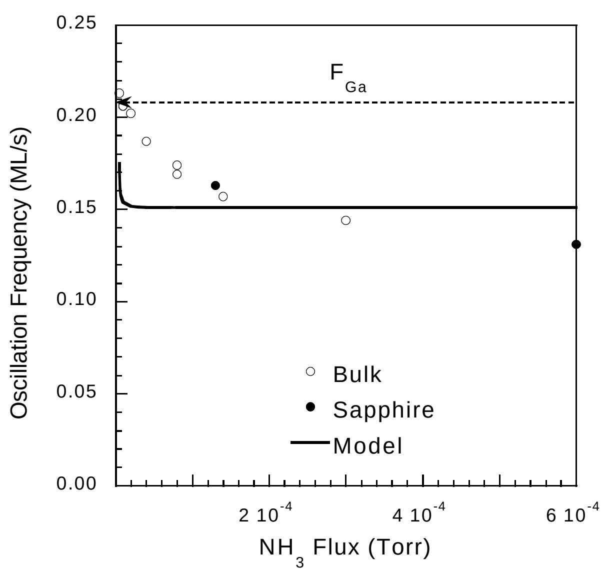


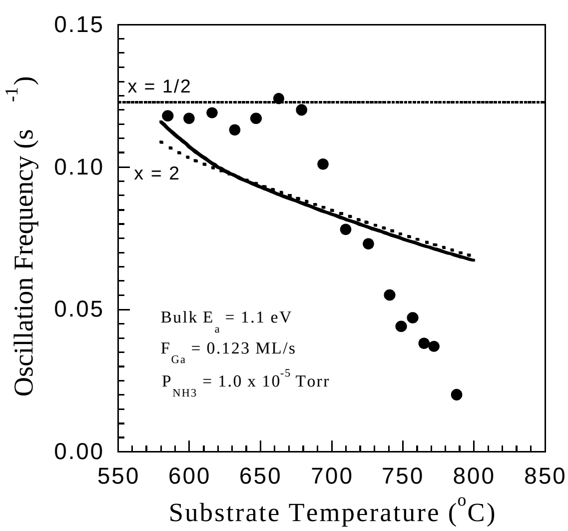
- best fit obtained with $x = 2$
- crossover relatively independent of f

Growth Rate Data and Model









- growth rates can be modeled qualitatively
- quantitative match not very good (depends on f)
- inhibitation term necessary
- qualitative agreement with RHEED data

Conclusions

- two surface terminations:
  gallided = unreactive
  nitrided = reactive

- gallided surface has weakly adsorbing site, surface diffusion

- nitrided surface is gallided by chemisorption via an intrinsic physisorption precursor state

- terminations and growth mode:
  gallided = step flow
  nitrided = island nucleation

- rate equation growth model:
  qualitatively good
  quantitative shortcomings