

Stripe formation close to a critical point: Au on W(110)

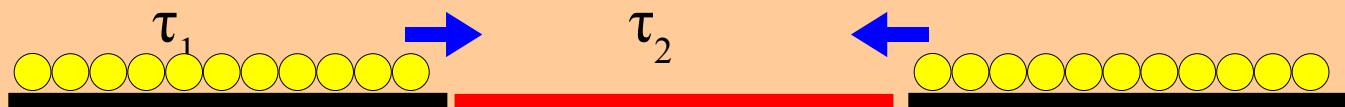
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Universidad Autónoma de Madrid, Spain
Sandia National Laboratories, USA



Stress-domain self-assembly

Competition between cost of making boundaries, and elastic interaction between the boundaries deforming the substrate and **lowering** the energy:

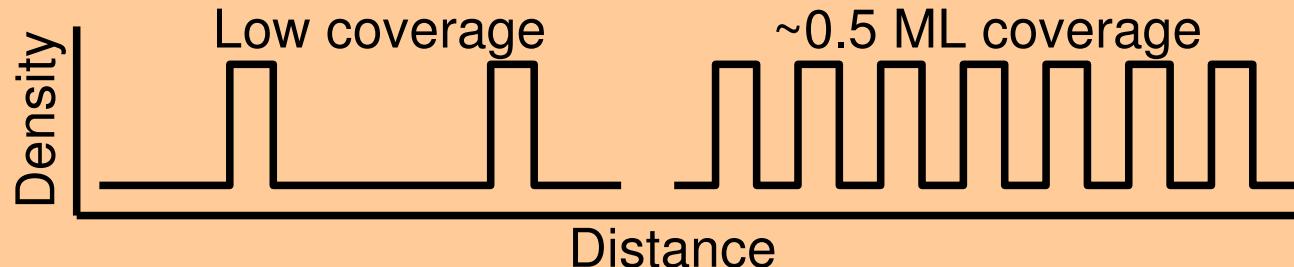


- Total energy per unit length of an array of domains, including the boundary energy,

$$E(l) = C_{boundary} - C_{elastic} \ln\left(\frac{2l}{\pi a}\right)$$

- There is a preferred length

$$l_0 = \frac{\pi a}{2} e^{\frac{C_{elastic}}{C_{boundary}} + 1}$$



O. L. Alerhand, D. Vanderbilt, R.D. Meade and J.D. Joannopoulos, *Phys. Rev. Lett.* **61** (1988) 1973

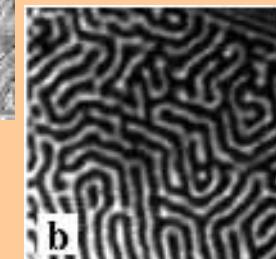
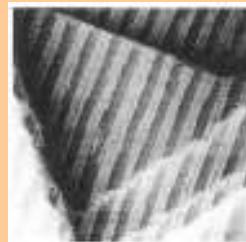
V. I. Marchenko, *Sov. Phys. JETP* **54** (1981) 605

<http://surfmooss.iqfr.csic.es>

Stress domains for self-assembly of patterns on surfaces

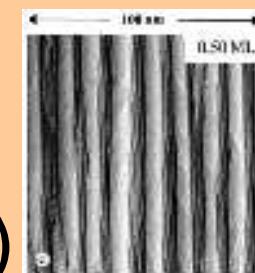
- Flat domains:

- O/Cu{110}-(2x1)O
- Si(100): original motivation
- Pb/Cu(111): best example so far



- Faceted Surfaces:

- Au(111) vicinals
- Ag-induced faceting of Cu(111)



P. Zeppenfeld et al., *Phys. Rev. Lett.* **72** (1994) 2737
O.L. Alerhand et al., *Phys. Rev. Lett.* **64**, (1990) 2406
S. Rousset et al., *Surf. Sci.* **422** (1999) 33
A. R. Bachmann et al., *Surf. Sci.* **526** (2003) L143
R. Plass et al., *Nature* **412**, (2001) 875
R. van Gastel et al., *Phys. Rev. Lett.* **91** (2003) 055503

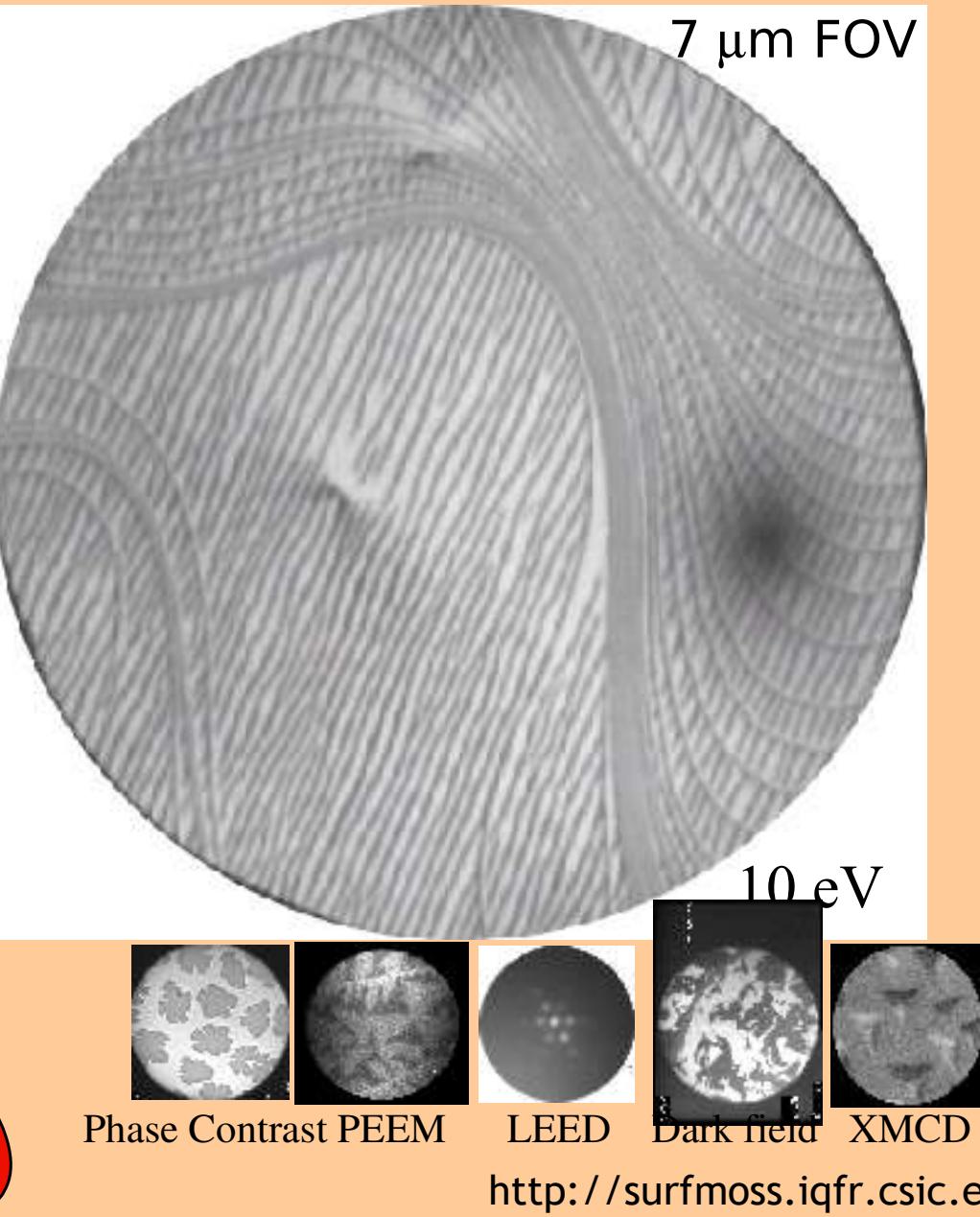
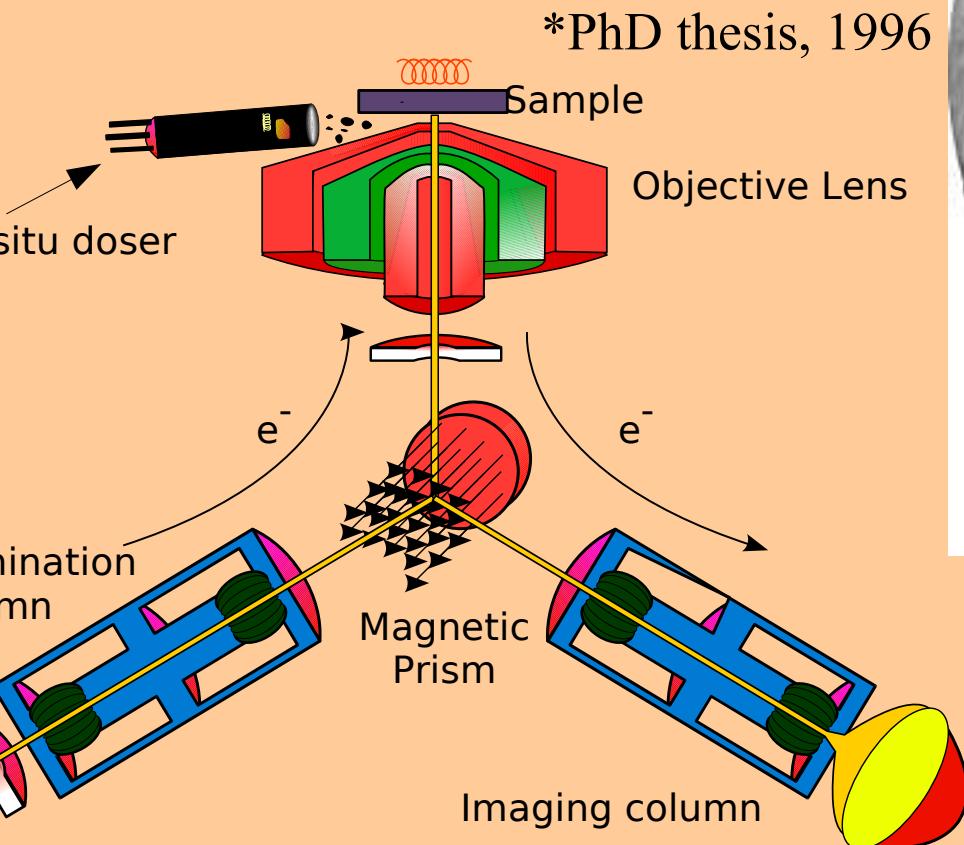
And some cases were it was assumed:

- Au(111) herringbone
- S/Ag/Ru(0001)
- N/Cu(100)



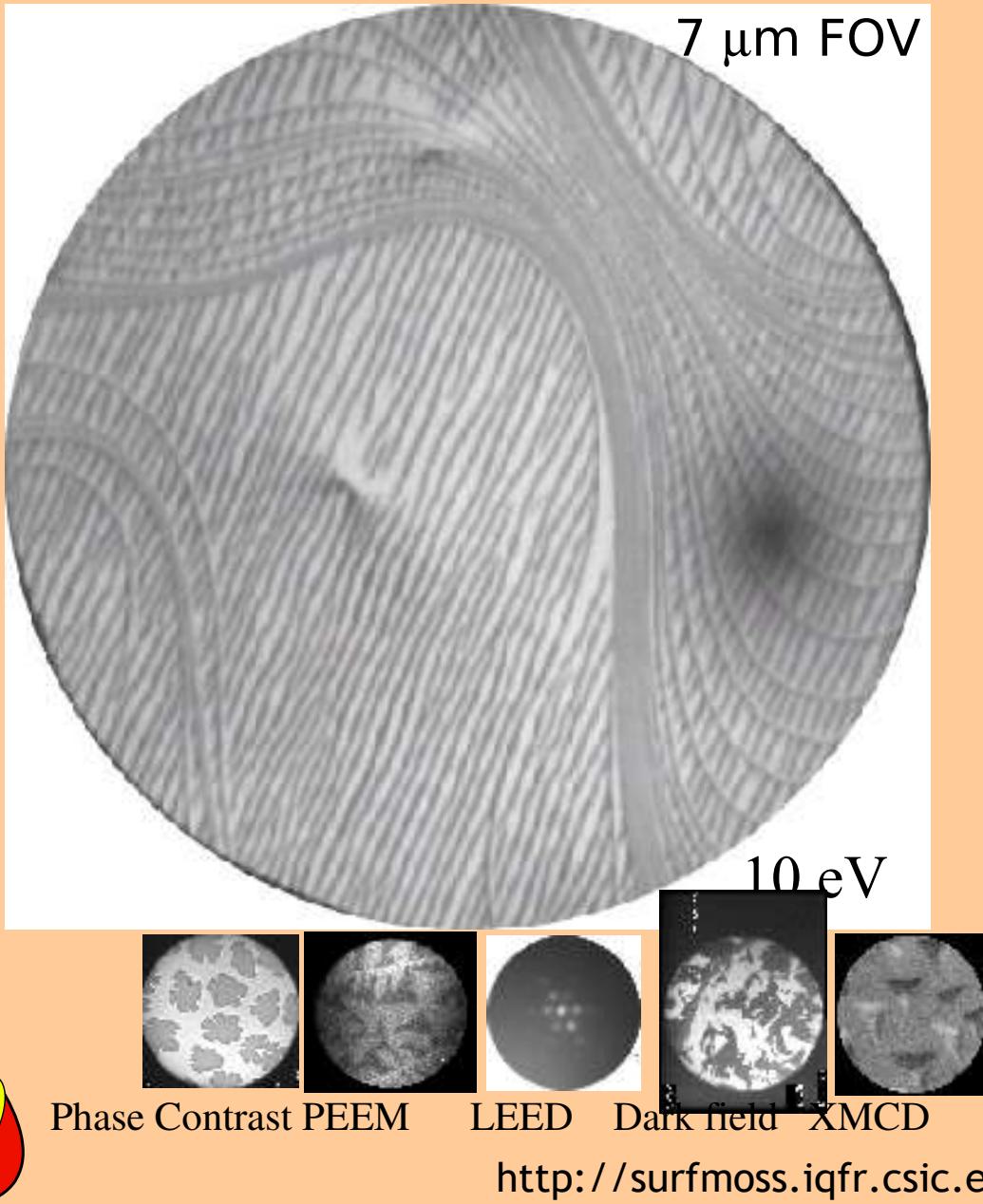
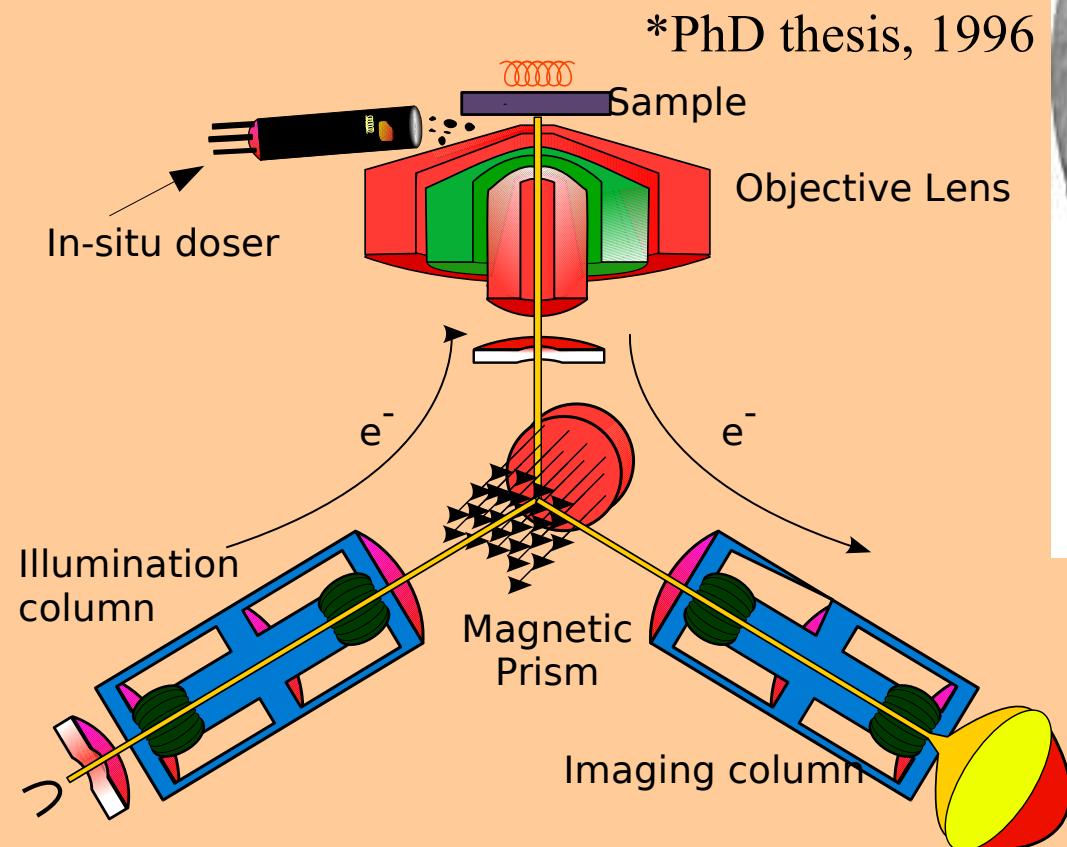
Stripes on Au/W(110) observed by LEEM

- A very simple system:
- Deposit Au at the appropriate temperature
- First reported by Thomas Duden and Ernst Bauer*



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Do the deposition at a higher temperature: breaking up the standard model

Unlike at lower temperatures, the periodicity does not seem to change much!

7 μm FOV



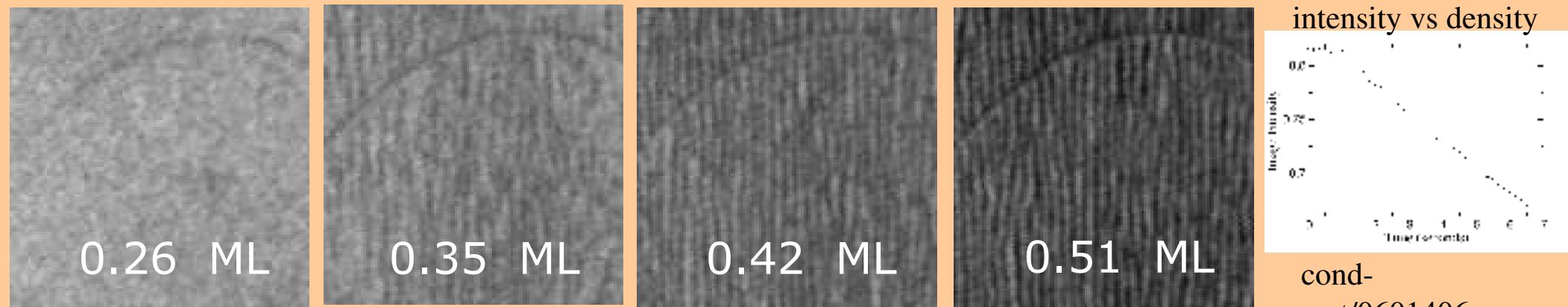
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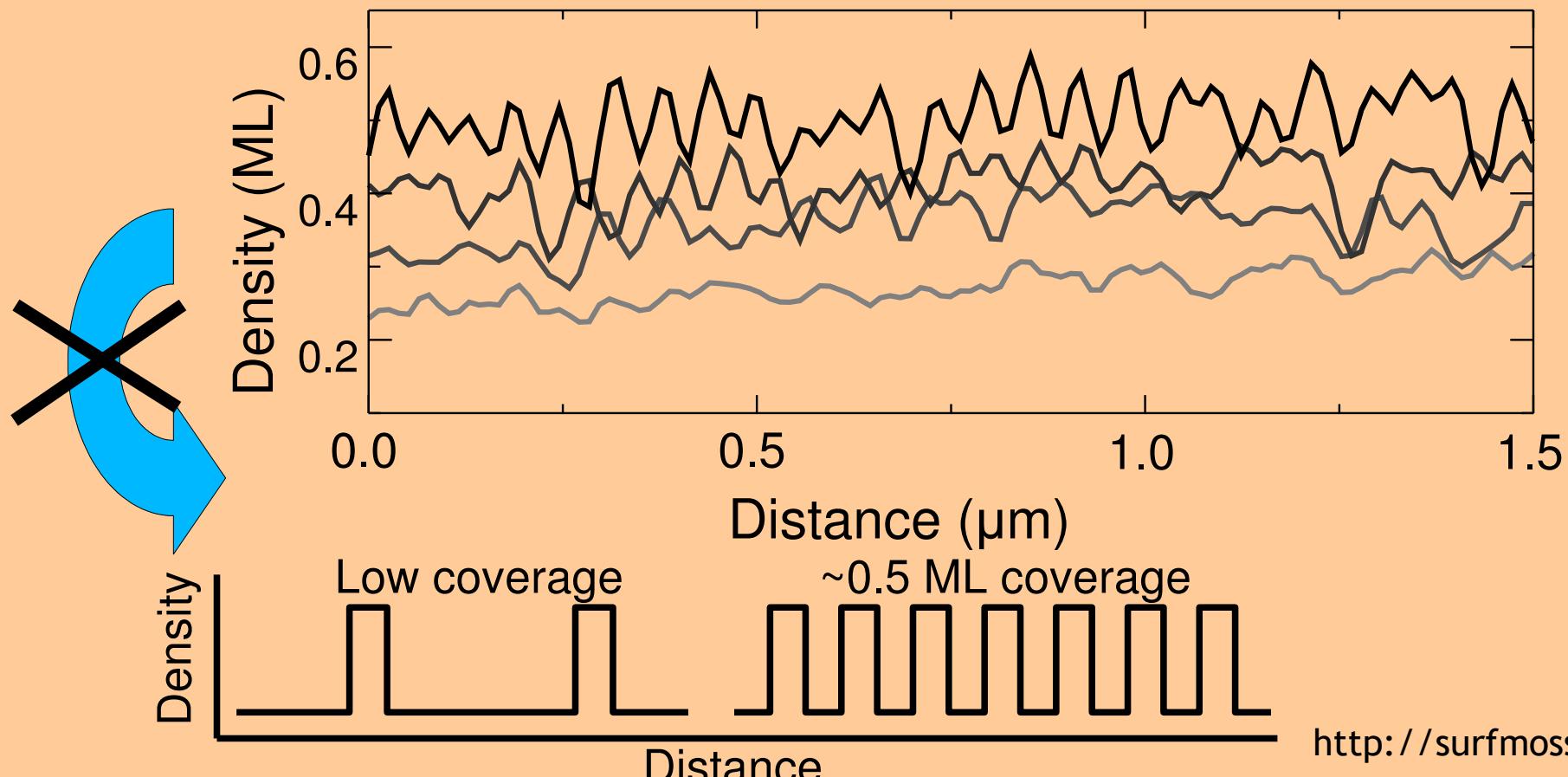
7 μm FOV



Evolution with coverage

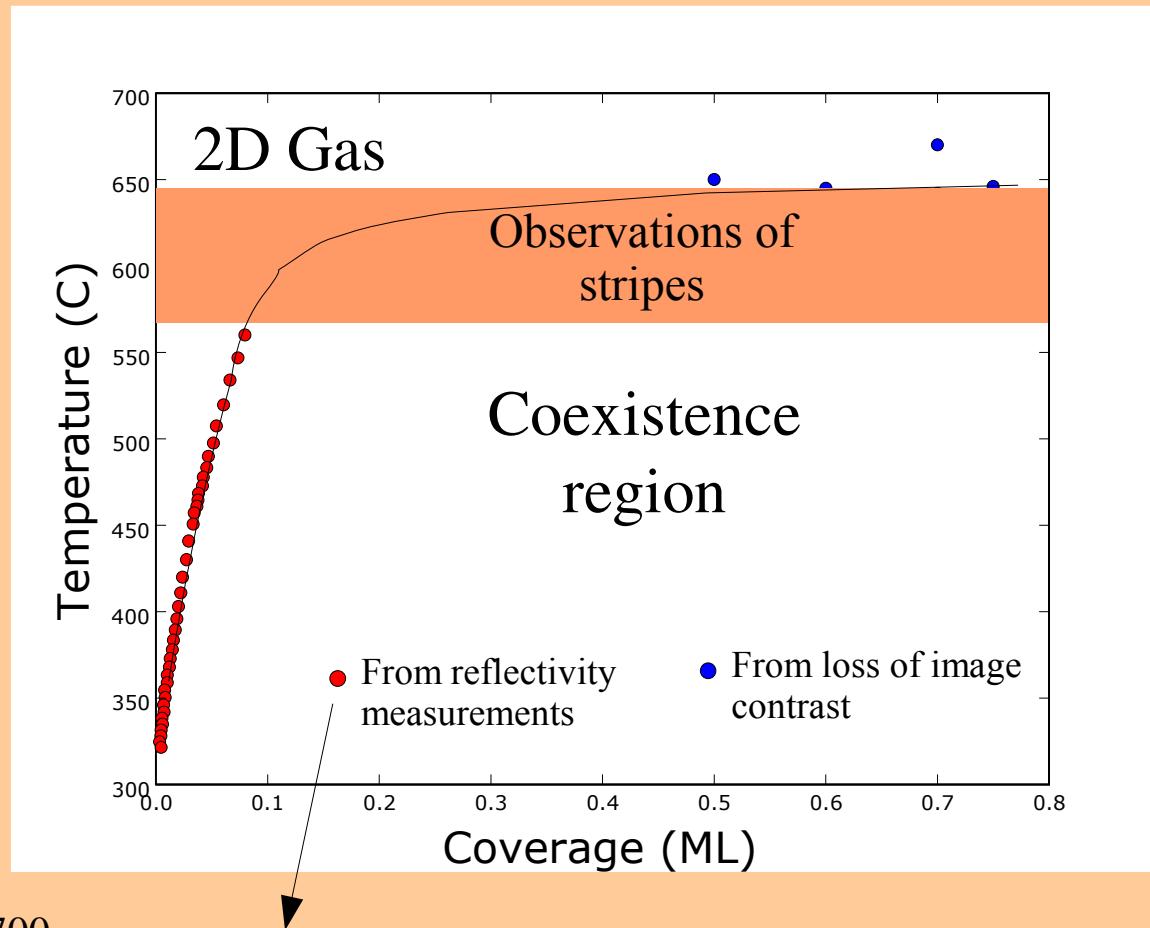
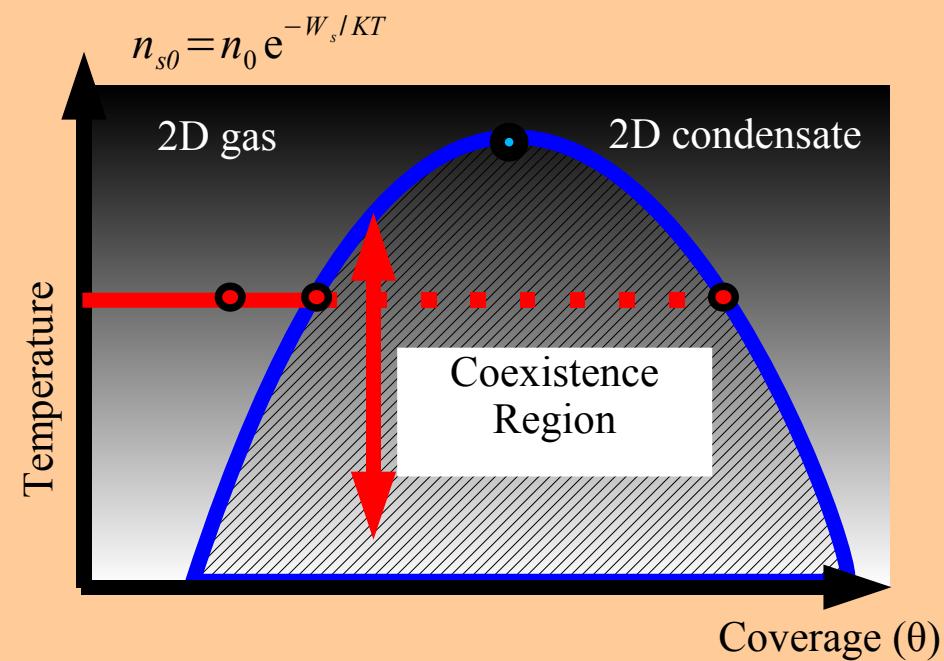


cond-
mat/0601406



We are close to the critical point...

Typical 2D phase diagram



J. Kolaczkiewicz and E. Bauer, *Surf. Sci.* **155** (1985) 700
J. Kolaczkiewicz and E. Bauer, *Surf. Sci.* **151** (1985) 333

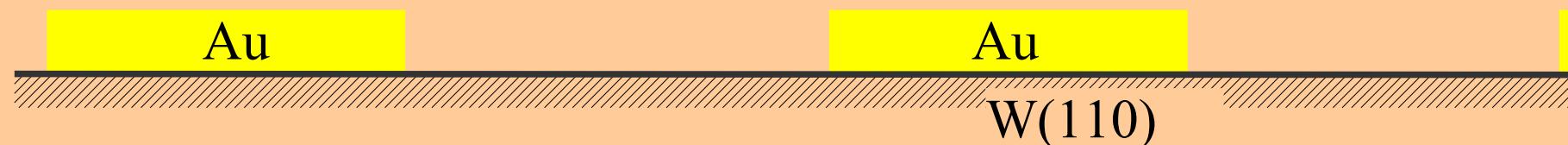
Juan de la Figuera, Norm C Bartelt, Kevin F McCarty,
Surf. Sci. **600** (2006) 4062 cond-mat/0601406

What is the problem?

- Up to now, we are assuming we have sharp boundaries:

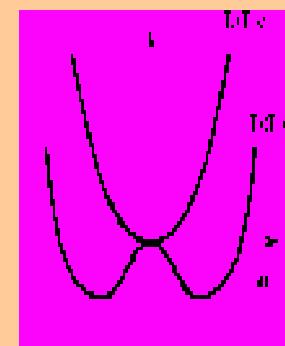
- compact condensed gold phase
- empty space between them

$$\lambda \approx e^{\frac{C_{boundary}}{C_{elastic}}} + 1$$



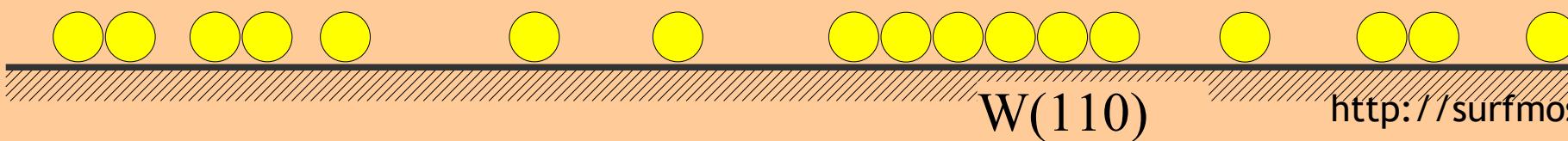
- But as we are not so far from the critical point, nothing is so distinct:

- we have a dense adatom gas in between (0.2 ML!), separated by not-so-compact condensed Au
- use a continuum model, with variable density $\phi = (2\rho - \rho_0)/\rho_0$



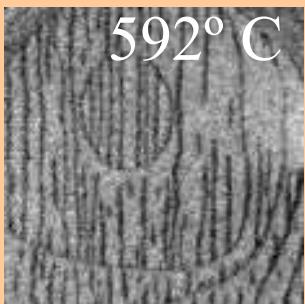
$$f[\phi(x)] = \int dx \left[-\frac{r}{2} \phi^2 + \frac{u}{4} \phi^4 + \frac{c}{2} |\nabla \phi|^2 \right] + g \int \int dx dx' \frac{\phi(x)\phi(x')}{(x-x')^2 + a^2}$$

Critical point Elastic interaction
Cost of boundaries

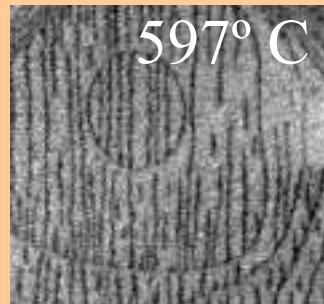


Change the temperature

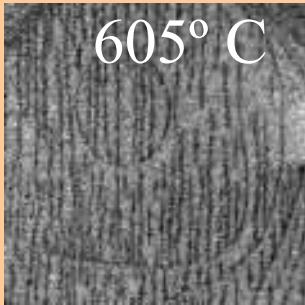
592° C



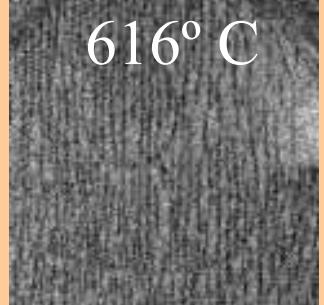
597° C



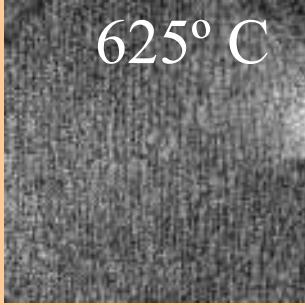
605° C



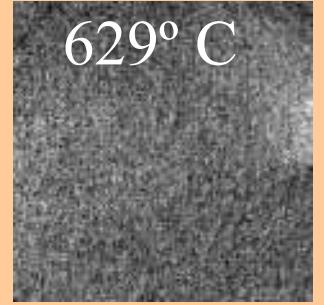
616° C



625° C



629° C

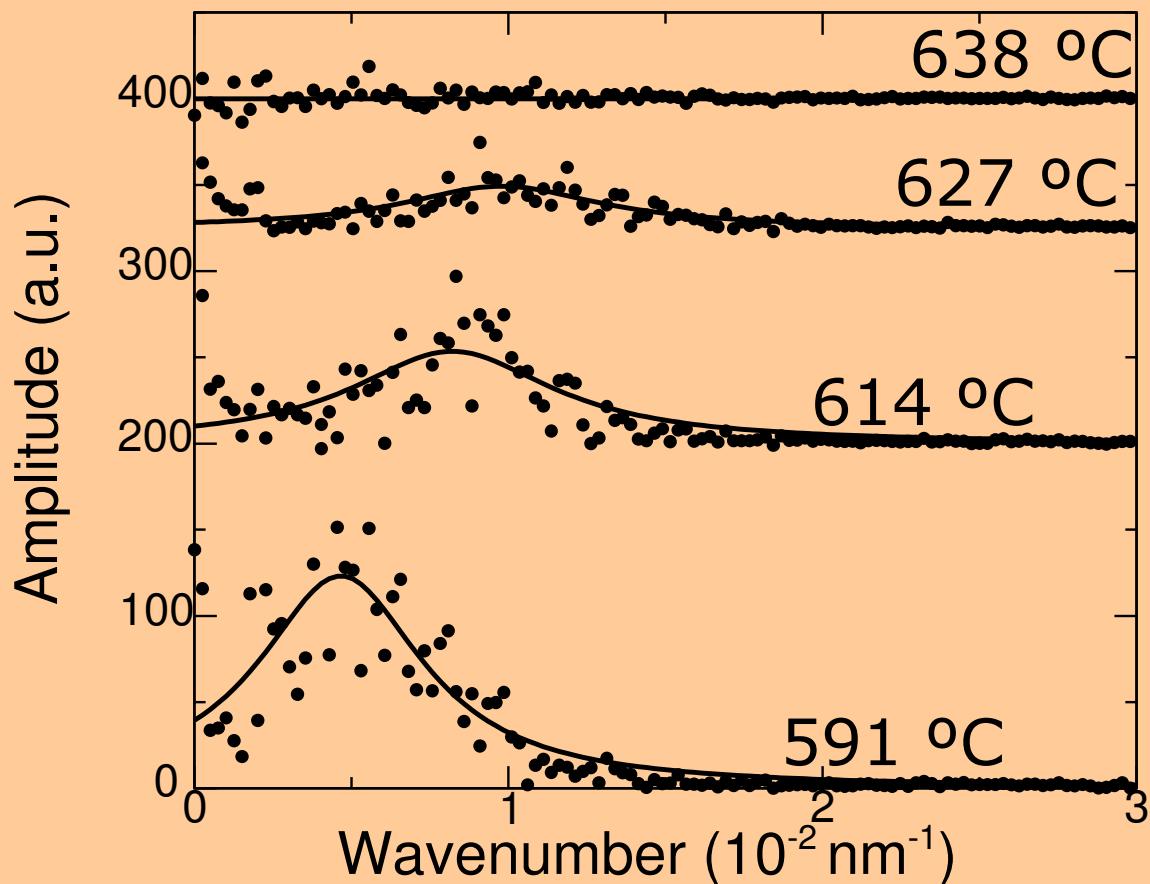
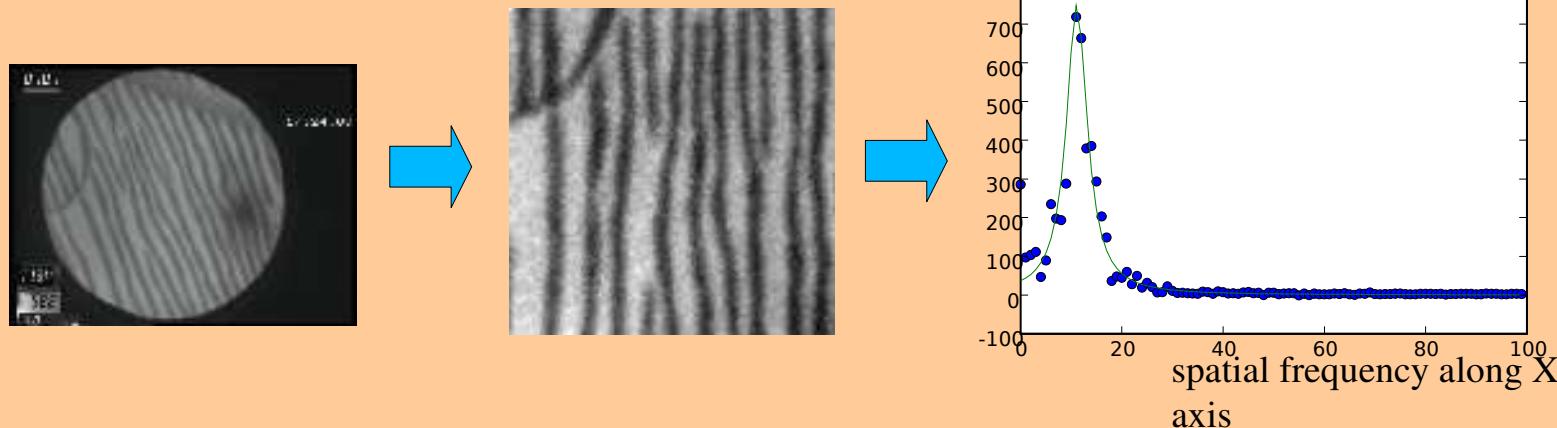


7 μm FOV



TEMPERATURE⇒

Measuring the pattern periodicity



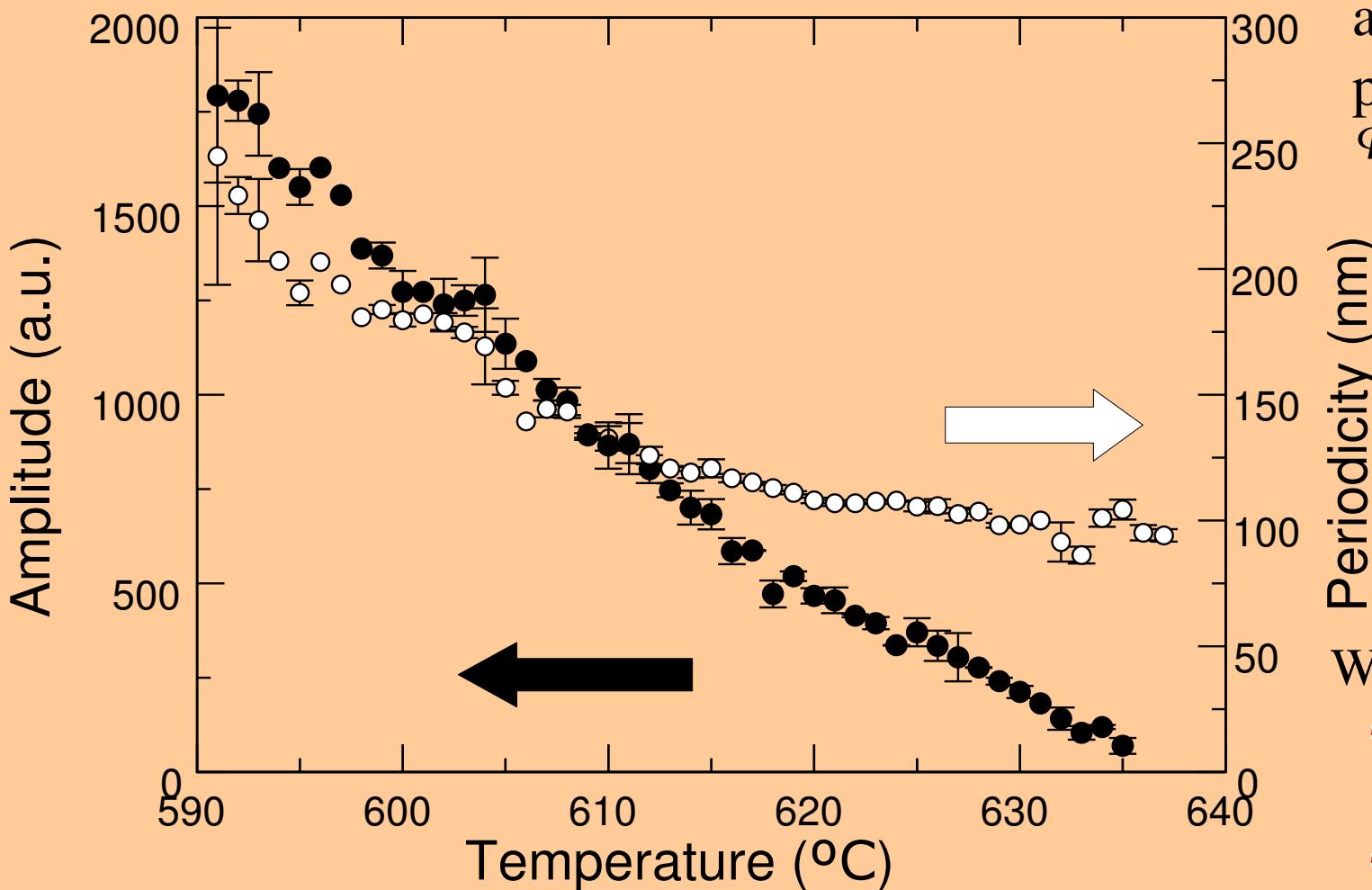
To extract stripe period from movie (between 20k and 30k frames):

- Rotate image (extract center area)
- Subtract background (unfocused)
- Perform a 2D FFT
- Extract a profile along k_x ($k_y = 0$)
- Average as many profiles as desired
- Fit the result to a lorentzian

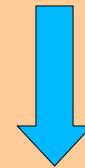
Limiting value of stripe periodicity!

Amplitude vs temperature: decreases steadily

Periodicity vs temperature: reaches a constant value



For the **diffuse boundary model**,
assuming a sinusoidal profile at high T:
 $\phi(x) = A \cos(2\pi/\lambda_c)$



$$\lambda_c = \frac{\gamma c}{g} \neq \dots$$

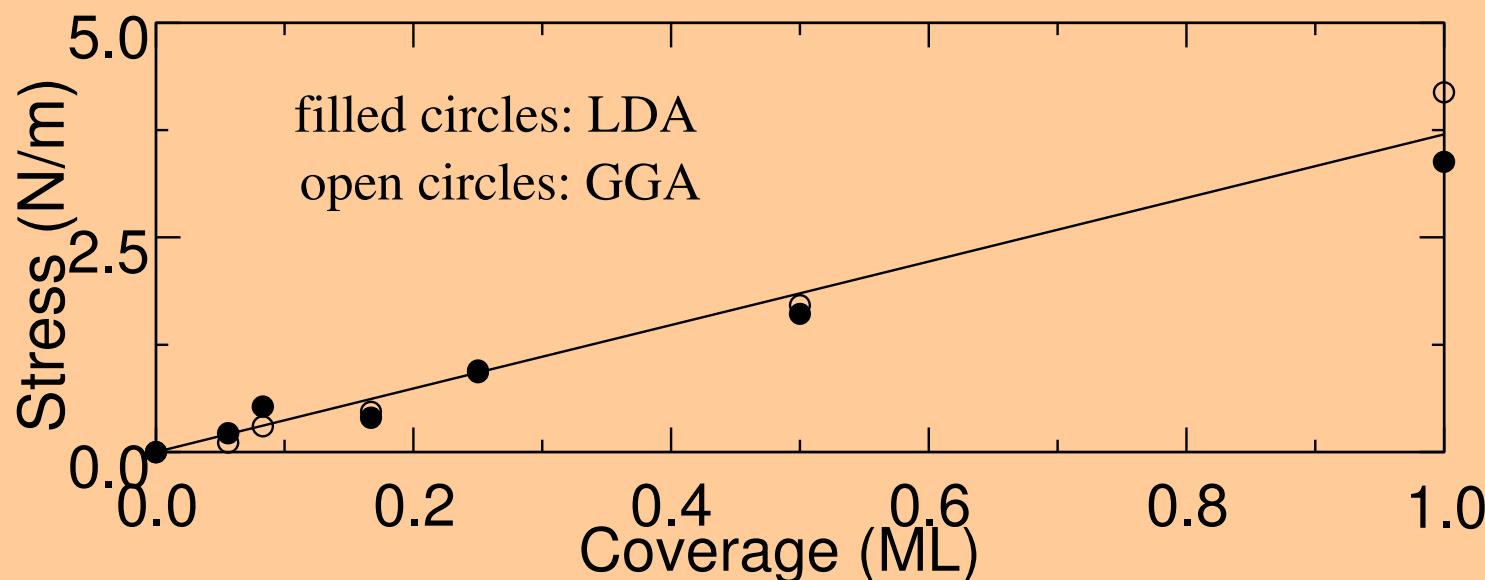
We need an estimate of:

- short range interaction
- long range (elastic) interaction

Long range elastic interaction

- Use DFT (VASP) to compute the (excess) surface stress as a function of Au coverage... $\Delta\tau$
- Use (non-isotropic!) elasticity theory to estimate the interaction for a given stress difference given the Au/W(110) stripes orientation: M F. Leonard, N. C. Bartelt, and G. L. Kellogg, *Phys. Rev. B* **71**, 045416 (2005).

$$g = (\Delta\tau)^2 M / 2\pi = 9.8 \times 10^{-12} \text{ J/m}$$

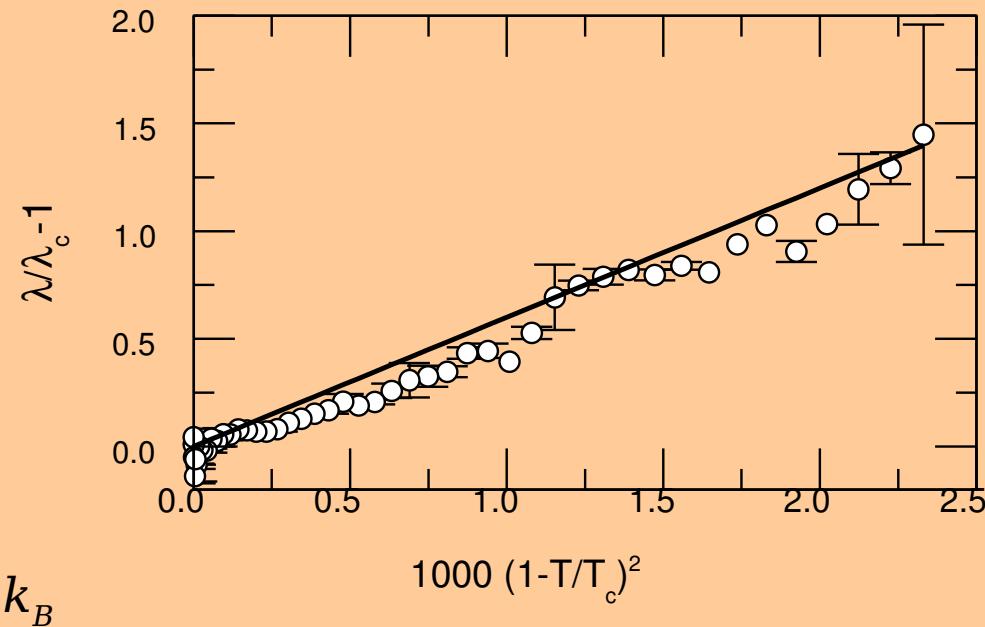


Short range interaction

- Study how stripe periodicity and amplitude change when approaching T_c
 - Extend the previous one-mode analysis to two modes
- Stripe periodicity close to T_c :

$$\lambda = \lambda_c \left[1 + \frac{\lambda_c^2}{\pi \Lambda \epsilon \pi^4} \left(\frac{a^2 r_* T_c}{c} \right)^2 \left(1 - \frac{T}{T_c} \right)^2 \right]$$

$$\frac{a^2 r_* T_c}{c} \approx 0.5$$



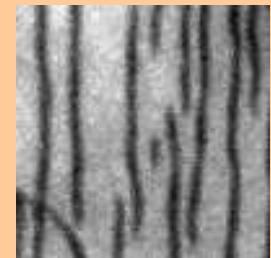
J. W. Cahn and J. E. Hilliard, *J. Chem. Phys.* **28**, 258 (1958)

$$a^2 r_* = 4 k_B$$

By fitting the previous dependence, we obtain $c \approx 8 k_B T_c$

$$\lambda_{c, theory} = \frac{2c}{g} \approx 20 \text{ nm}$$

Summary



- We have characterized the stripe formation of Au on W(110):
 - Observations at high T are incompatible with the sharp-boundary model
 - Non-constant density in components of stripes
 - Limiting value of periodicity
- The results can be understood within a model *with diffuse boundaries*:
 - The prediction is a linear dependence on material properties

We expect modulated patterns to be prevalent close to critical points at surfaces!!

The people that does the work!

the experimentalists



Kevin F. McCarty

This work is supported by the DOE Basic Energy Science program and by the Spanish Ministry of Education and Science

arxiv 0804.1273, accepted Phys. Rev. Lett.

and the theory people

Norm C. Bartelt

Roland Stumpf



Francois Leonard



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