Distinctive Features in Growth on Vicinal Cu(100): Understanding the Role of Impurities by Calculating Key Energies and Simulating Morphology

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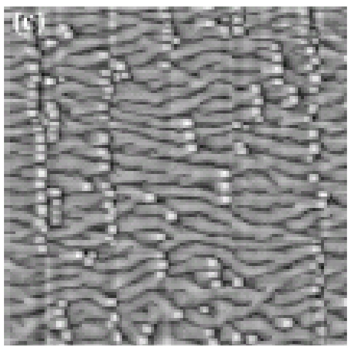
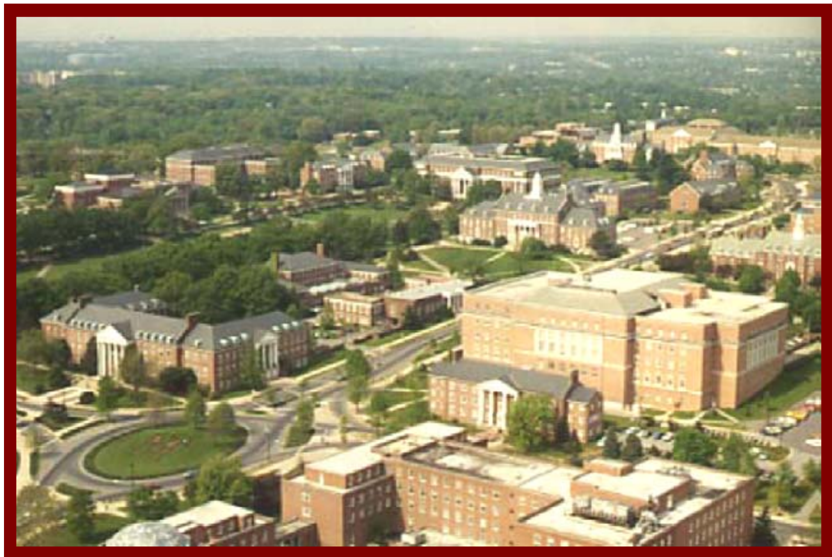
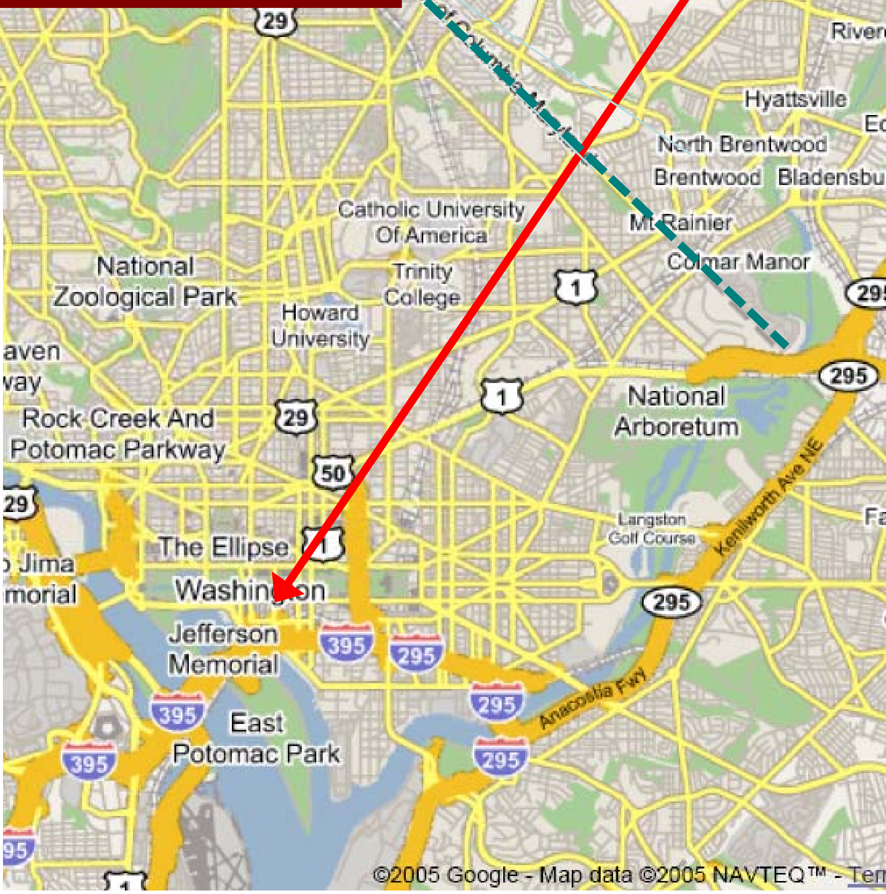


Maroutian,…,Ernst, PRB 64 ('01) 165401

- Impurities (co-deposited) can account for unusual $\lambda_m(F)$ behavior (not Bales-Zangwill) of meandering instability on vicinal Cu [Ernst group] and for distinctive pyramidal nanostructures.
- KMC predicts key energies of such impurities; with DFT we survey various possibilities and identify the likely species.
- Survey of morphologies at 40 ML and submonolayer
- Description in terms of capture-zone distributions & their characteristic exponent ϱ.

Primary support: NSF MRSEC grant DMR 05-20471





UM is "inside the Beltway".

UM ↔ DC center:

~ 14 km.

3rd n^n Max Born Symposium $4^4 = 256$

- Born 11 Dec. 1882 Breslau (Wrocław) to Margarete Kauffmann (<textile wealth) & Gustav Born (*med. prof. embryology*, son of Marcus Born né Buttermilch, also MD), [unobservant, assim.] *Jewish* (D's 3rd largest)
- *Mother died at age 4*; *oldest child* (sister & step-sister); *frail, shy,retiring*
- U. Breslau, Heidelberg U., U. Zürich, 1904 to U. Göttingen for Ph.D. & Hab.('09), contact with Klein, Hilbert, Minkowski, Runge, Schwarzschild, Voigt; also Larmor & Thomson (U. Cambridge); student with von Kármán, Ewald, Toeplitz, Hellinger
- 1913 married Hedwig Ehrenberg (Jewish father converted to Lutheran when married), Hedi baptized; mother-in-law hounded Born to convert); 3 children inc. Irene (mom of Olivia Newton-John)
- 1915 prof. at U. Berlin, spurn Haber (b. Wrocław) offer to work on gas warfare; friends with A. Einstein; stint in army

Nobel laureates

Notable students:

M. Delbrück
W. Elsasser
F. Hund
P. Jordan
M. Goeppert-Mayer
L. Nordheim
J.R. Oppenheimer
V. Weisskopf

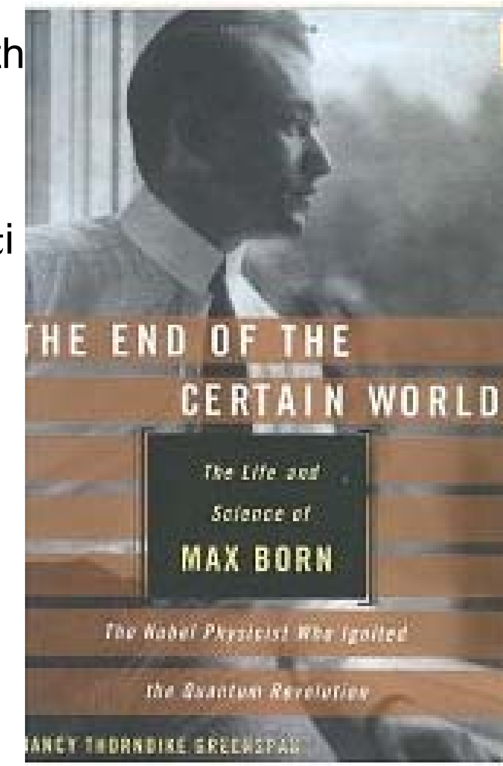
Notable assistants:

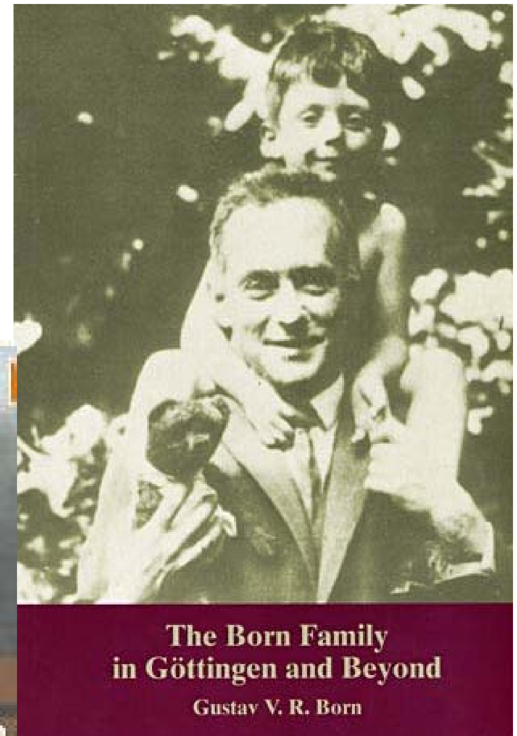
E. Fermi
W. Heisenberg
G. Herzberg
P. Jordan
L. Rosenfeld
E. Teller
E. Wigner (TLE great-grand-advisor)
K. Fuchs
W. Heitler
F. Hund
W. Pauli
O. Stern

- 1921 prof & Inst. Director U. Göttingen, also got chair for Franck
- Grew depressed: family lost wealth due to war & inflation, rising anti-Jewish, and Hedi had long-term affair with Göt. mathematician Gustav Herglotz (& Born knew)
- 1933 emigrated since avowed pacifist & stripped of Ph.D. & Prof. due to Jewish race Stokes Lecturer, U. Cambridge; Hedi back to Göt. for months
- 1936 Tait Prof. at U. Edinburgh, British citizen, FRS ('39)
- 1954 Nobel Prize w/ W. Bothe (Heisenberg: 1932); *X* P. Jordan: Nazi
- 1954 retired to Bad Pyrmont (Hedi's choice, where she had rested ere marriage & Quaker mtgs., 100 km NW of Göttingen
- 1955 signed Russell-Einstein manifesto
- 1970 died, buried in Göttingen cemetery with Nernst, Weber, von Laue, Planck, Hilbert

tombstone:

$pq-qp = h/2\pi i$





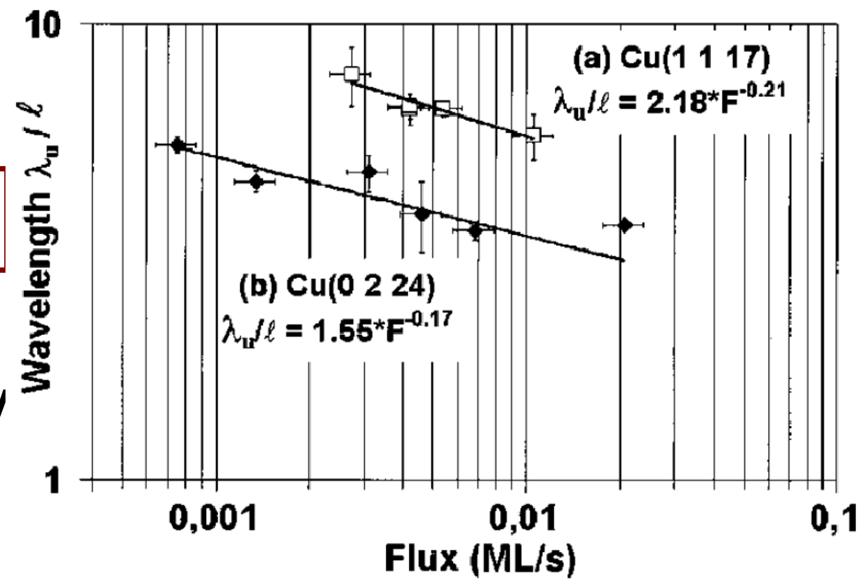
Crater Born on moon,
d = 15km,
at 6.0°S 66.8°E

Motivations: What role of E-S barrier effect during growth ? Why does λ (F) of Cu meandering instability differ from B-Z ?

Experiment Cu(1 1 n) & Cu(0 2 24)

Driving force of meandering instability = ***F*** (flux)

- Meandering period = $\lambda_{exp't} \propto F^{-\gamma}$, γ_{expt} **≈ 1/6-1/5**



Stabilizing force of the meandering instability

Diffusion mechanisms

- Meandering λ has Arrhenius form

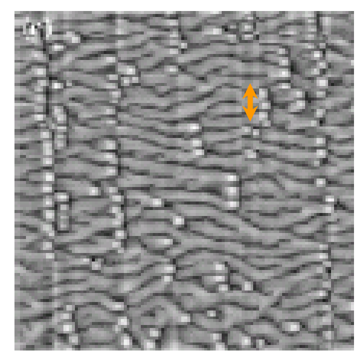
Linear theory, Bales & Zangwill

Meandering wavelength: $\lambda_{th}=(D_m/F\langle\ell\rangle^2)^{1/2}$,

D_m: edge diffusion

γ_{BZ} **= 1/2**

Cu (1 1 17)

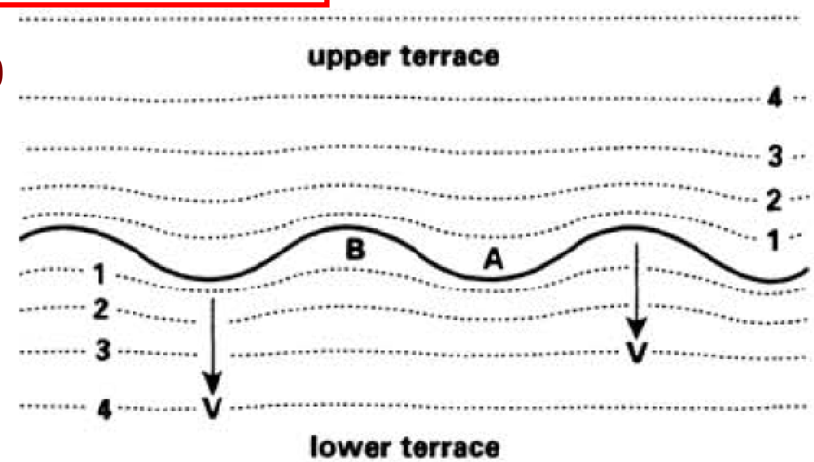


Maroutian et al., PRB 64 ('01) 165401

Why not Ehrlich-Schwoebel (BZ), KESE or USED?

▪ **Measured meandering length =** $\lambda_{exp} \propto F^{-\gamma}$, $\gamma \approx$ **1/6-1/5**

Linear theory, Bales & Zangwill, PRB 41 ('90) 5500

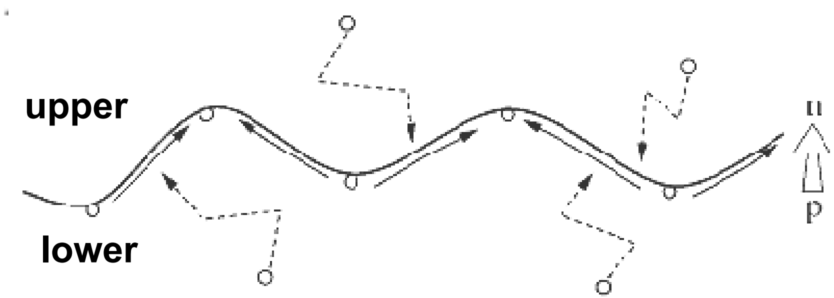


Meandering wavelength: $\lambda_{th}=(D_m/F\langle\ell\rangle^2)^{1/2}$,
D_m: edge diffusion

$\lambda_{th} \propto F^{-\gamma}$, γ **= 1/2**

▪ For kink Ehrlich-Schwoebel effect (KESE)
[**O. Pierre-Louis**,…,TLE, PRB 82 ('99) 3661]:

$\lambda_{th} \propto F^{-1/4}$, i.e., γ **= 1/4**



but KESE predicts that zig-zag ⟨100⟩ steps are stable, contrary to exp't.

▪ For unhindered step edge diffusion (USED) **[F. Nita & AP, PRL 95 ('05) 106104]:**
γ **= 0.14-0.20**, small kink barrier gives good morphologies, but would need very small ES barrier, contrary to evidence (0.1–0.25 eV) and no pyramids.

Kinetic Monte Carlo of model with 2 chemical species

$P = \nu_o \exp(-E/k_B T)$: probability of a diffusion event

$E = E_d^{p} + n\epsilon^{pq} + (E_{ES} + E_{iES})$: total energy

p,q ≡ ***s*** (substrate/adatom), ***i*** (impurity)

ν_o : hopping frequency

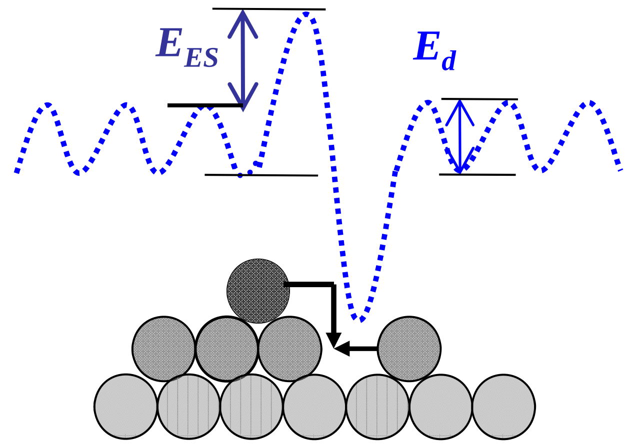
$n = 0, 1, 2, 3$: first neighbor

E_d : diffusion energy

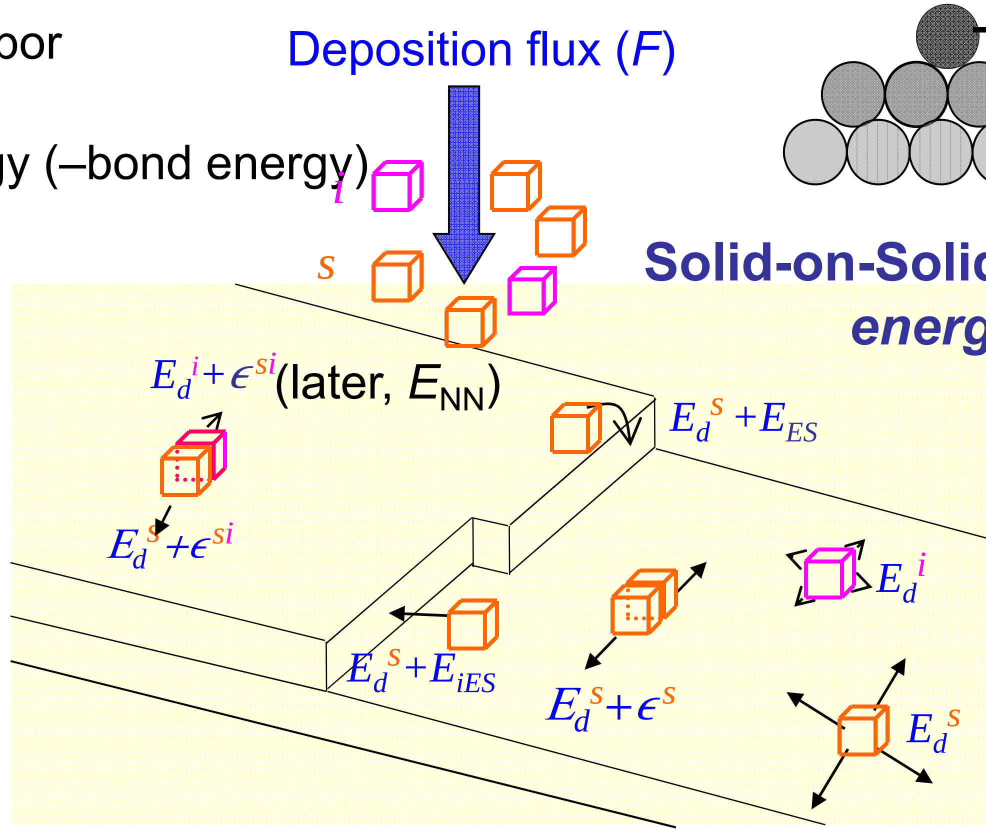
ϵ: attachment/det. energy (–bond energy)

E_{ES} : ES barrier

E_{iES} : inverse ES



Solid-on-Solid (SOS) model
energy barriers



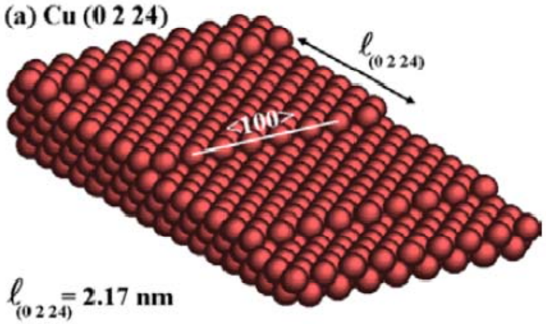
What impurities?

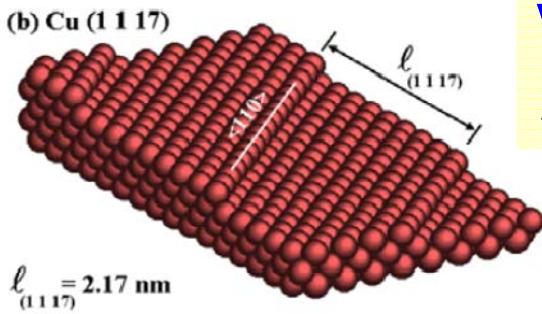
- *lower mobility*
- *small conc(%),*
- *higher binding*

Neglects:

- rapid edge running
- vacancy transport (sliders)

Vicinal Cu: experiment [Néel et al., J.Phys: CM 15('03)S3227] vs. simulation





Pyramids (square bases):

- intrinsic (vacancies)?
- **2-particle model?**
- extrinsic (impurities)?

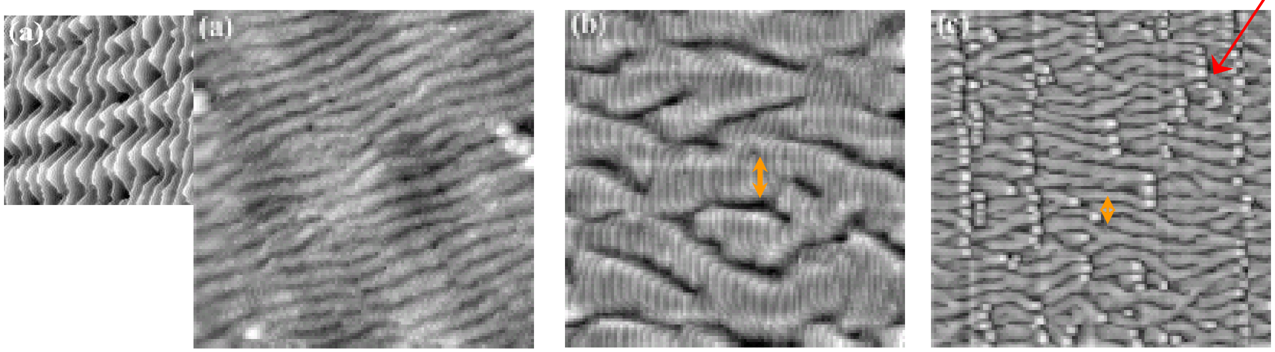
⇩

Impurities

Exp't

STM

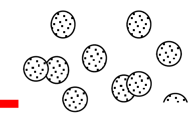
Cu (0 2 24) | Cu (1 1 17) | Cu (1 1 17)



(135nm x 135nm) F=3 x 10^{-3} ML/s

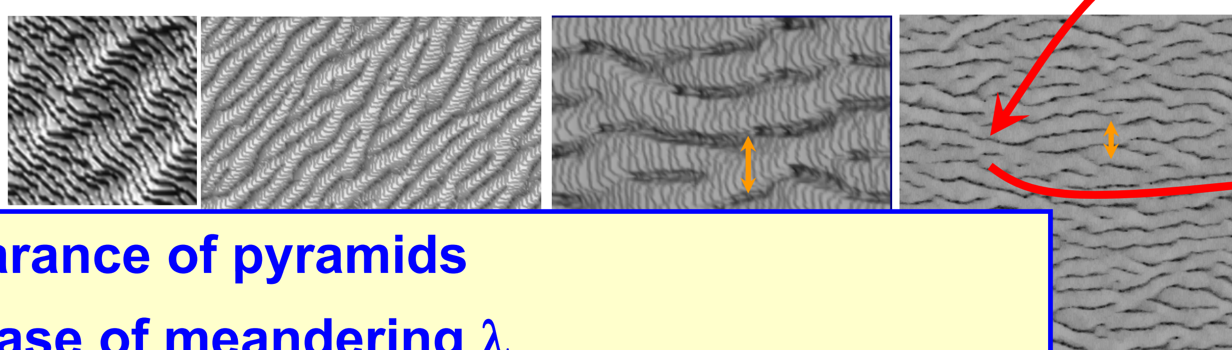
(85nm x 85nm) F=5 x 10^{-3} ML/s

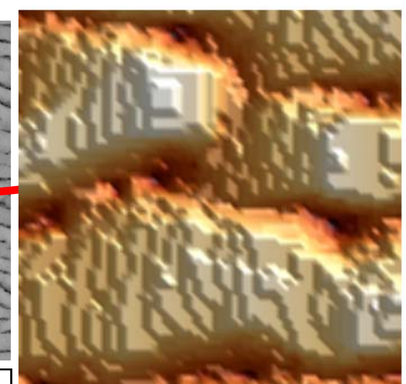
(400nm x 400nm) F=2 x 10^{-2} ML/s



E_d^i=0.6eV, ϵ^{si}=0.18eV

Sim.





- **Appearance of pyramids**
- **Decrease of meandering λ**

800x800, T=250K, F=5e-3, E_{ES}=0.10, Ed=0.4,Ea=0.15, L=06, 20 ML

240x240, T=280, **F=5 e-3**, E_{ES}=0.07, Ed=0.4,Ea=0.12, L=8, 20 ML

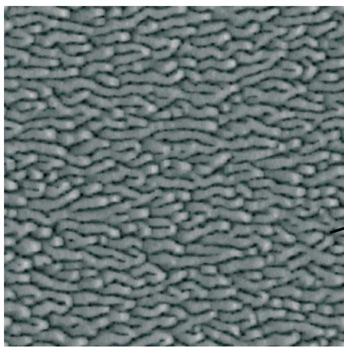
1000x1000,T=280, **F=5e-2**, E_{ES}=0.07,Ed=0.4, Ea=0.12, L=8, 40 ML

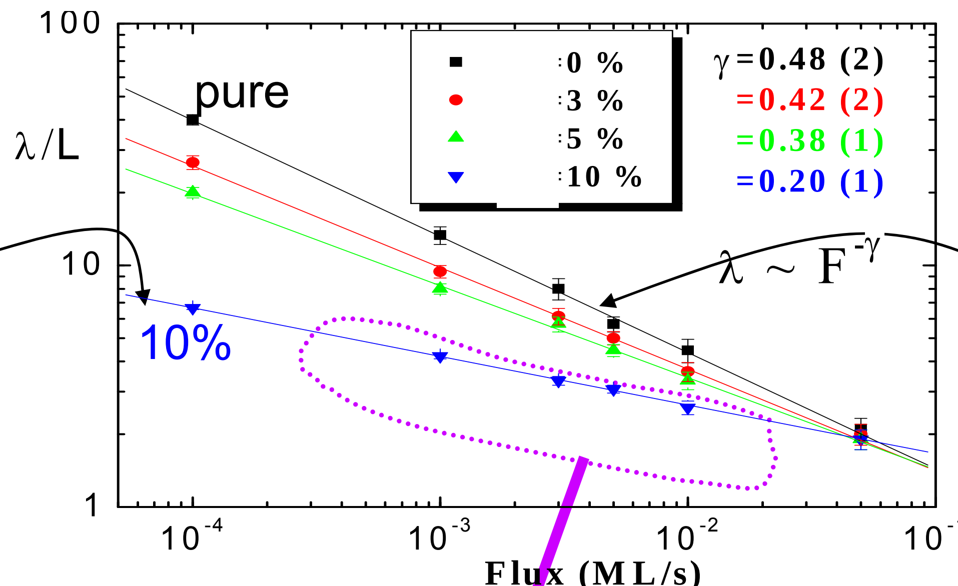
Posited impurities reconcile experiment and theory

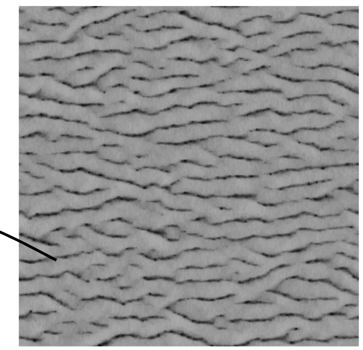
Impurities → exp'tal morphology & variation with F
Meandering: $\lambda_{sim} \propto F^{-\gamma}$, γ **=1/2-1/5**

Embedded impurities can induce mounds, cf. Co on Cu(001). R. Pentcheva & M. Scheffler, PRB 65 ('02) 155418; O. Stepanyuk, N. N. Negulyaev, A. M. Saletsky, W. Hergert, PRB 78 ('08) 113406

Sim.

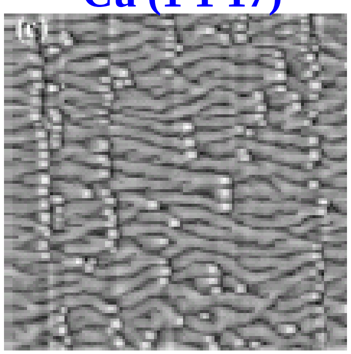




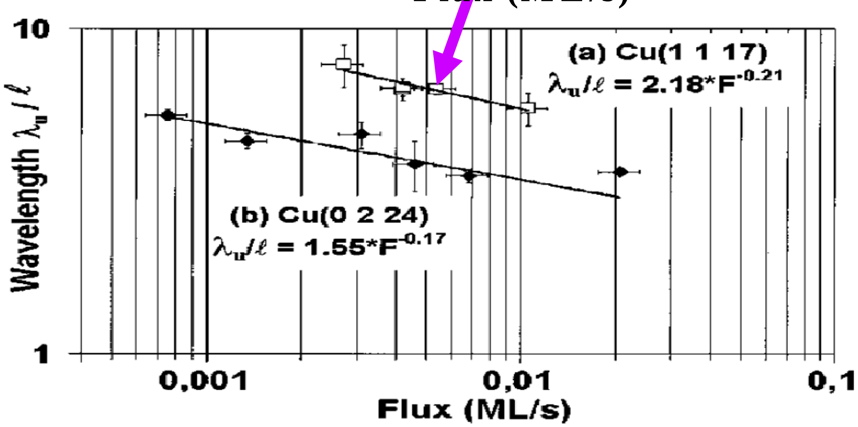


Cu (1 1 17)

Exp't

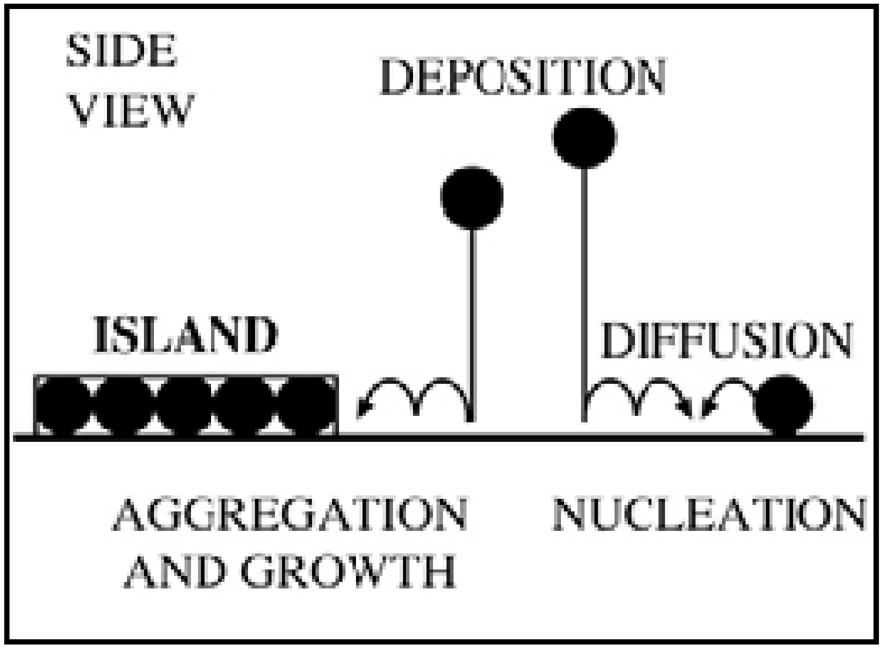


Maroutian et al., Phys. Rev. B 64(2001)165401



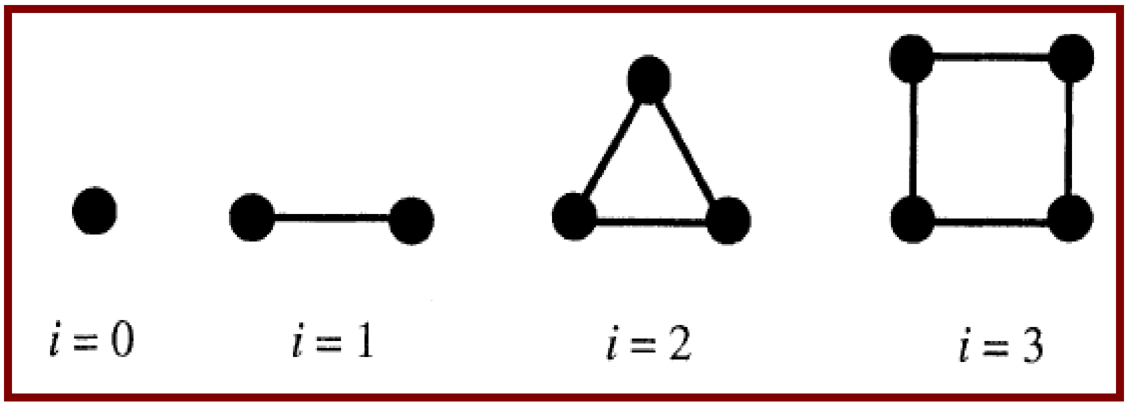
NB: 2% OK!

Description of deposition and island growth



J.W. Evans *et al*., Surf. Sci. Rept. 61 ('06) 1

- Atoms deposited randomly
- Then diffuse till they meet
- Nucleate island, which grows
- But small islands can break up

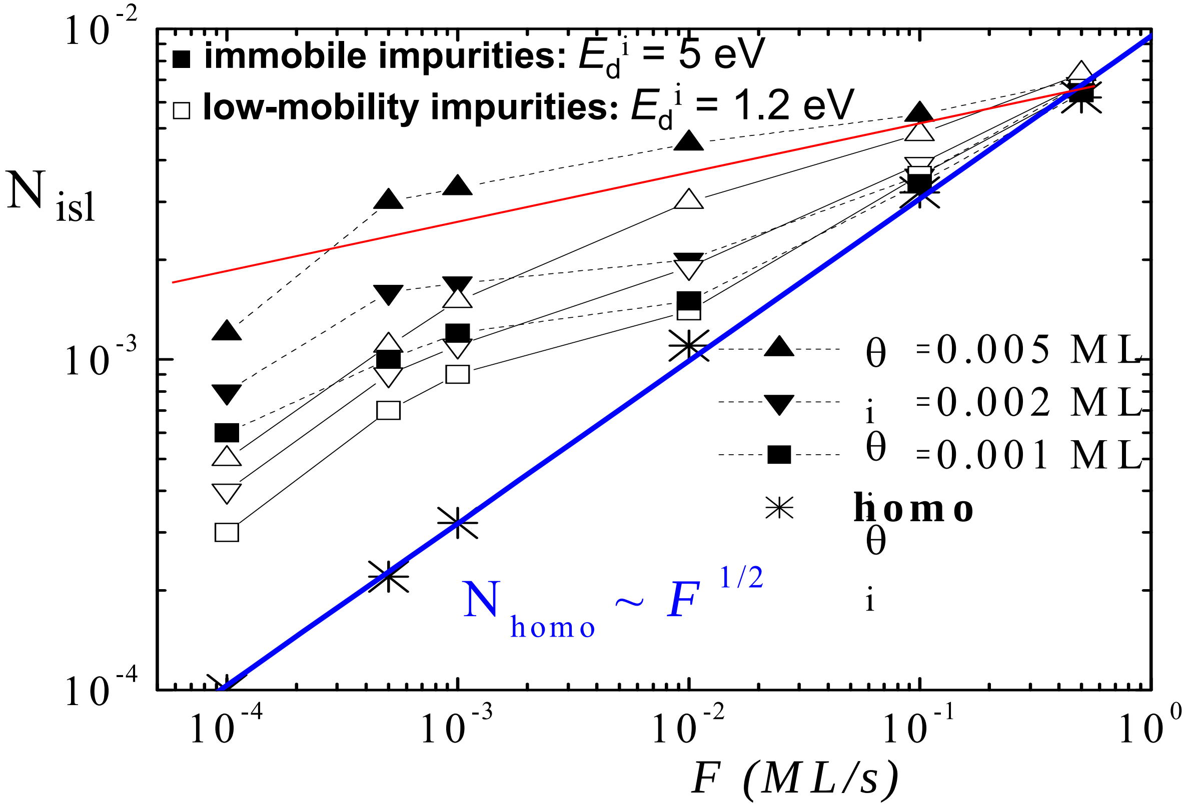


i*+1 atoms: smallest stable island:** ***critical nucleus

So *i* is size of largest unstable cluster

Effect of impurities on island density (diffusion length)

400x400, T=500 K, θ_s**=0.1 ML**, E_d^s=1.0 eV, E_d^i=1.2(**5**) eV
ϵ^{ss}=0.3 eV, ϵ^{si}=0.4 eV, ϵ^{ii}=0 eV



N_d : *islands density*
homo : *homoepitaxy*

$N_{homo} \sim F^{\chi}$

$\chi = 1/2$

$\chi = 1/6$

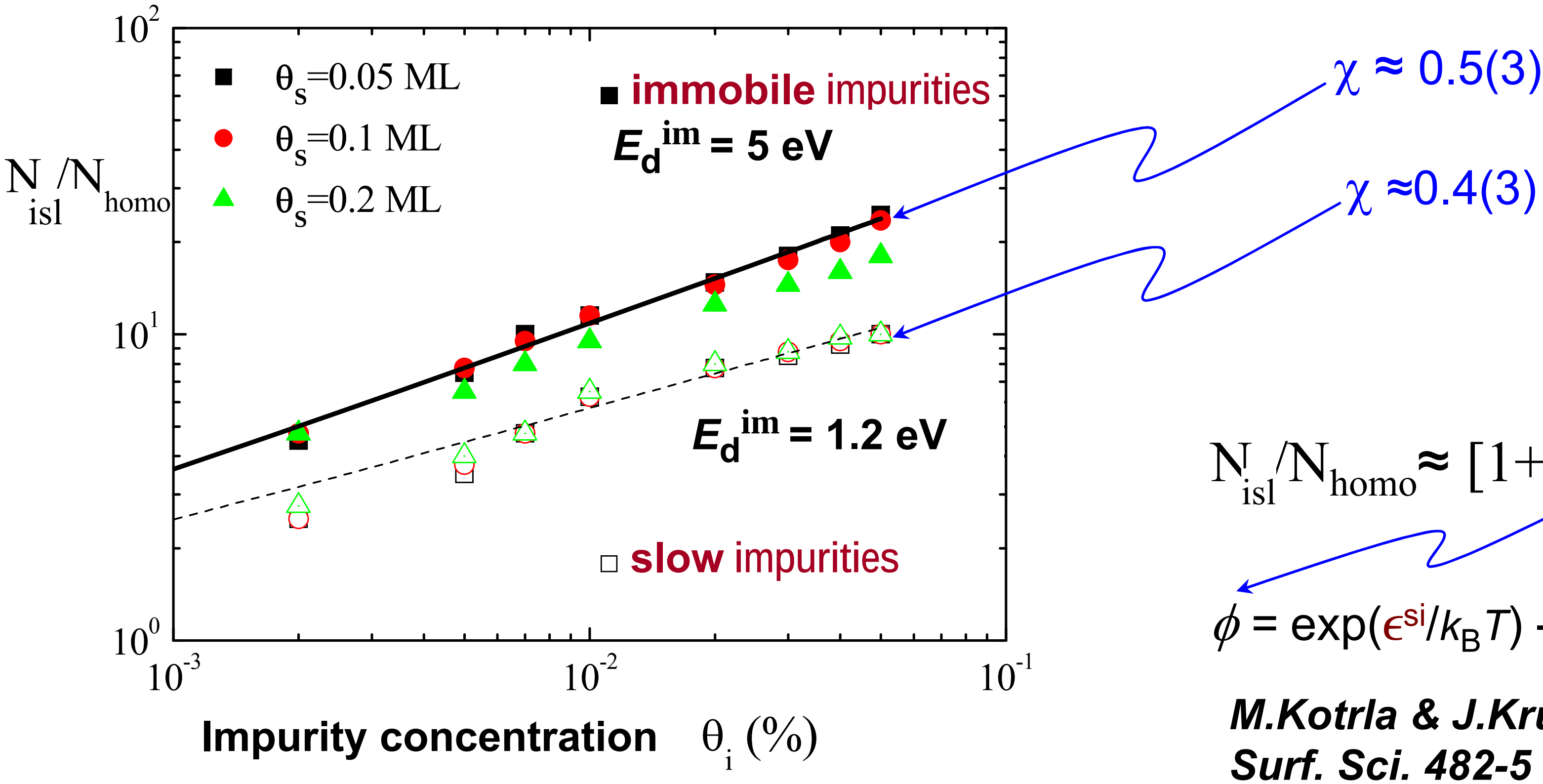
Impurities (θ_i) decrease dependence of island density (diffusion length) on *F*

Effect of impurities on island density

$N_{homo} \sim (F/D)^{\chi}$ $\chi = i/(i+2)$

i : *critical nucleus size*

N_d : *island density*
homo : *homoepitaxy*

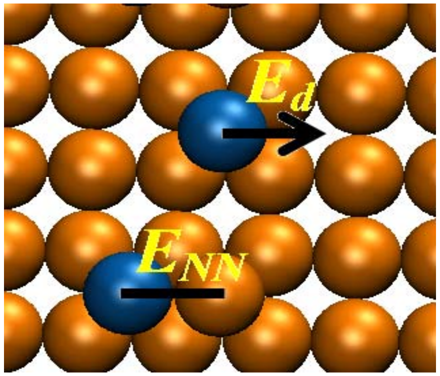


$$N_{isl}/N_{homo} \approx [1+\theta_i \phi]^{\chi}$$

$$\phi = \exp(\epsilon^{si}/k_B T) - 1$$

M.Kotrla & J.Krug, Surf. Sci. 482-5 ('01) 840

Island density N depends on the binding energy between adatoms and impurities (ϵ^{si})



KMC $\Rightarrow E_{NN} \gtrsim 1.2 \times 0.35$ eV
$E_d \approx 1.6 \times 0.56$ eV

Impurity Sets

$E_{NN}^{\text{imp-imp}}$ insignificant

	Element	E_{NN} (eV)	E_d (eV)	
	Cu	**0.350**	**0.564**	
vapor-phase	O	-0.337	0.775	$E_{NN} < 0$
	C	-0.251	1.827	
	S	-0.119	0.900	
full or empty *d*-band	Ag	0.277	0.390	$E_{NN} \lesssim E_{NN}^{Cu}$
	Sn	0.307	0.432	
	Zn	0.312	0.314	$E_d \lesssim E_d^{Cu}$
	Al	0.422	0.493	
incipient magnets?	Pd	0.343	0.698	$E_{NN} \approx E_{NN}^{Cu}$
	Ni	0.384	0.795	
	Si	0.386	0.862	$1.2 \lesssim E_d/E_d^{Cu} \lesssim 1.5$
mid-transition elements	Co	0.414	0.891	$1.2 \lesssim E_{NN}/E_{NN}^{Cu} \lesssim 1.8$
	Fe	**0.444**	**0.909**	
	Mn	**0.474**	**0.879**	$E_d \approx 1.6 \times E_d^{Cu}$
	W	**0.639**	**0.913**	

VASP-GGA

PAW-PBE

400eV cut-off

4x4x14supercell

6 atomic layers

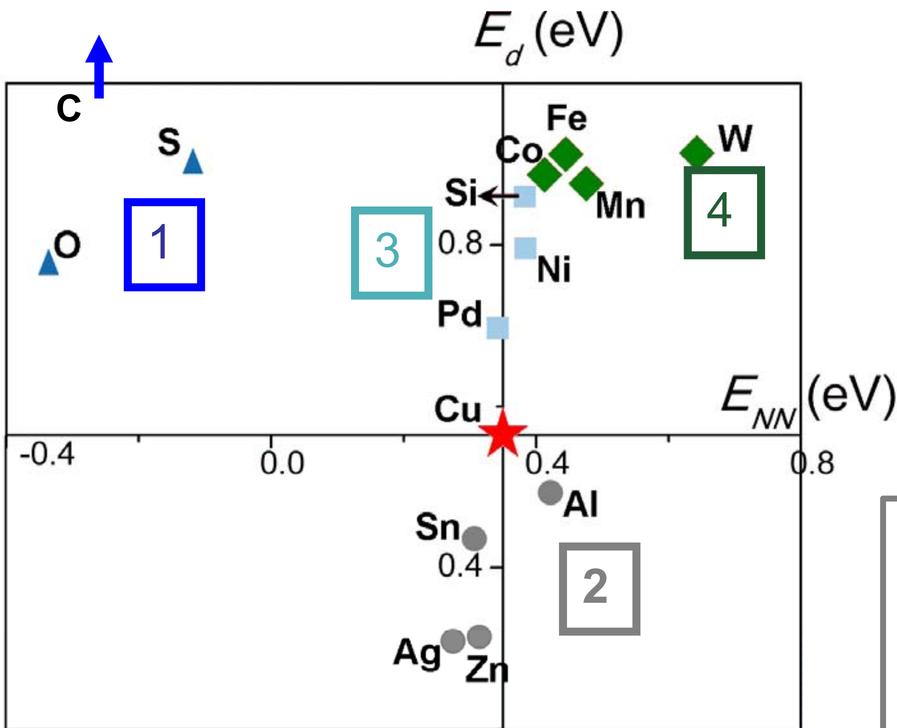
(5x5x1) **k** mesh

Which of these??

Graph of Impurity Sets

vapor-phase

full or empty *d*-band



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incipient magnets?

mid-transition elements

Effect of impurities in step-flow regime

γ = 0.45 (5) for pure Cu

$\lambda \propto F^{-\gamma}$

40 ML at F = 0.05 ML/s

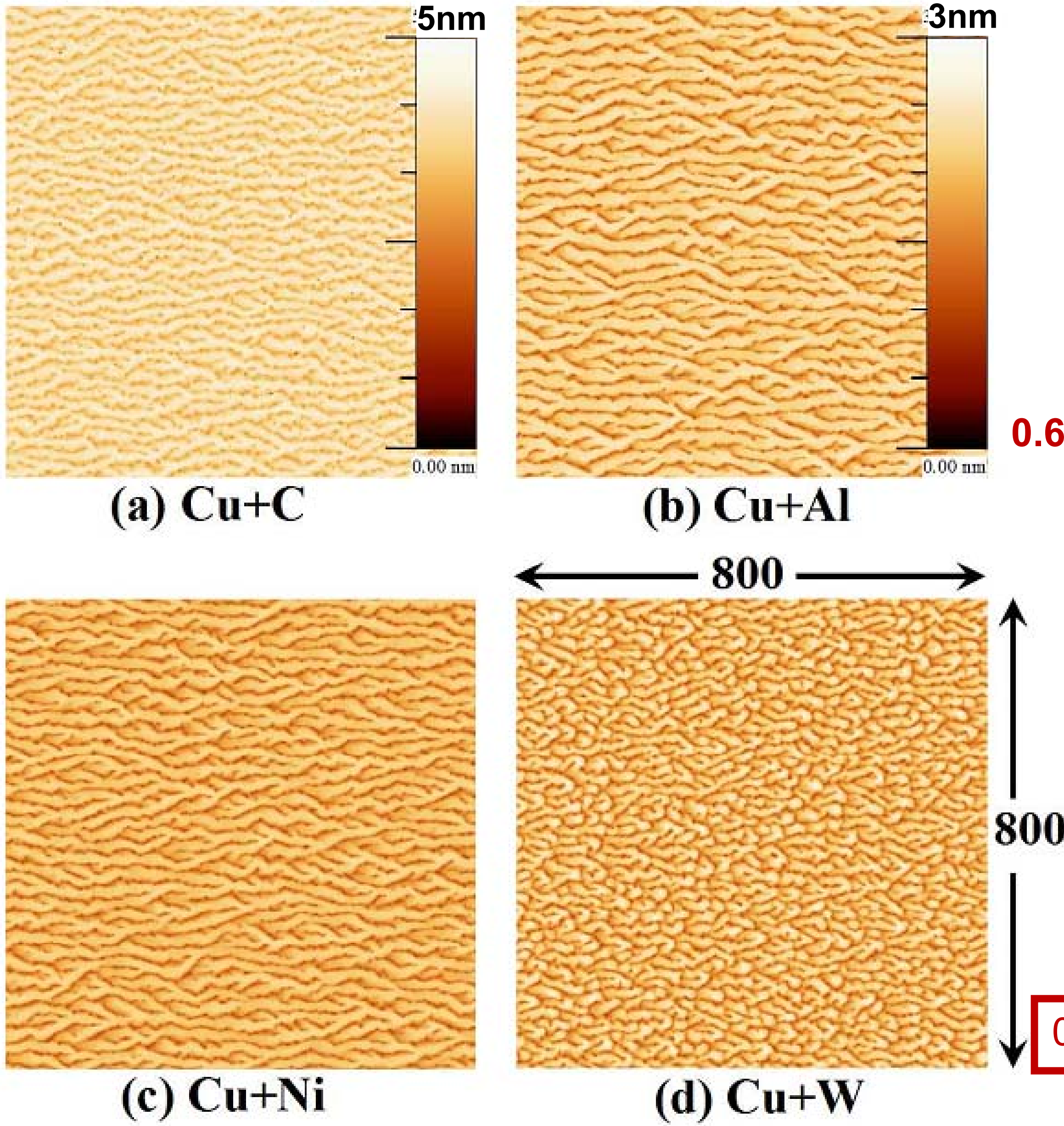
Cu + 2% impurity (co-dep)

0.35(6)

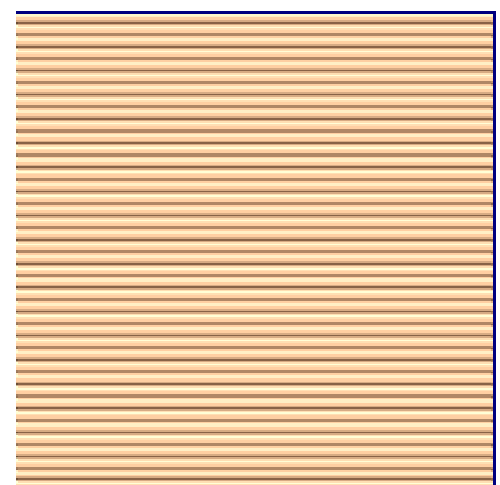
0.62(2)

0.43(6)

0.17(2)

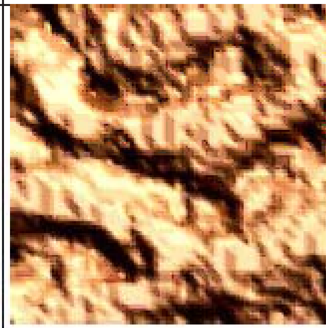
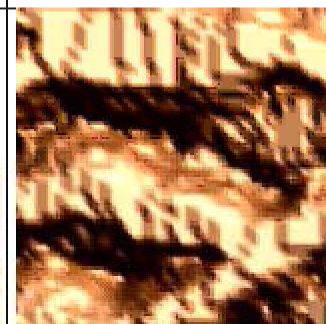
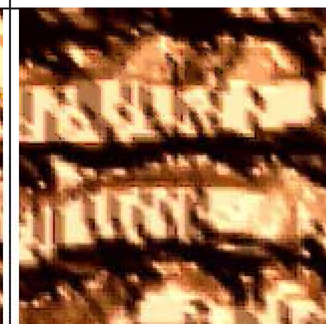


pure Cu



Cu + 2% Fe

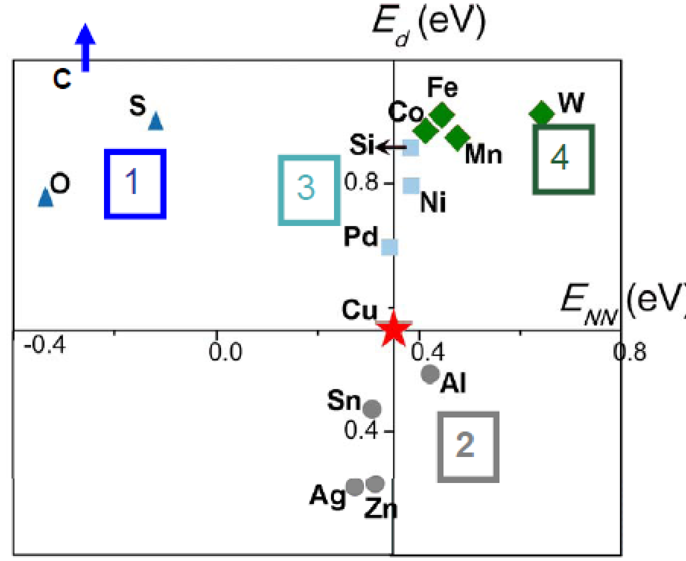
Estimates of γ ($\lambda_m \sim F^{-\gamma}$) and possibility of pyramid formation

Imp.	Cu	C (Set 1)	Al (Set 2)	Ni (Set 3)	W (Set 4)
γ	0.45 ± 0.05	0.35 ± 0.06	0.50 ± 0.06	0.41 ± 0.05	0.17 ± 0.02
Zoom View					

2% codeposited impurities

zoomed: 7% of previous images

40ML, F=0.05ML/s at T=425K



Why tungsten (W) from this set of impurities?

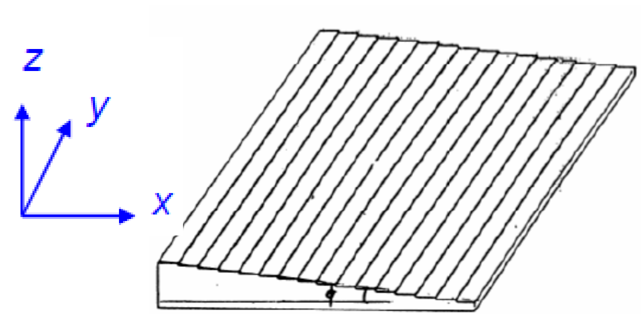
- W has best energies
- W has proper value of γ
- Mn unlikely to be part of apparatus, so Fe or W
- W heating element used in experiment (T. Maroutian)
- In experiment, pyramids began to appear for $F > 10^{-2}$ ML/s
- As raise T to raise F, more W from wire

Low W vapor pressure, not sure if direct sight to sample (B. Poelsema)
But perhaps H coats W, hampering sticking. (T. Seyller)

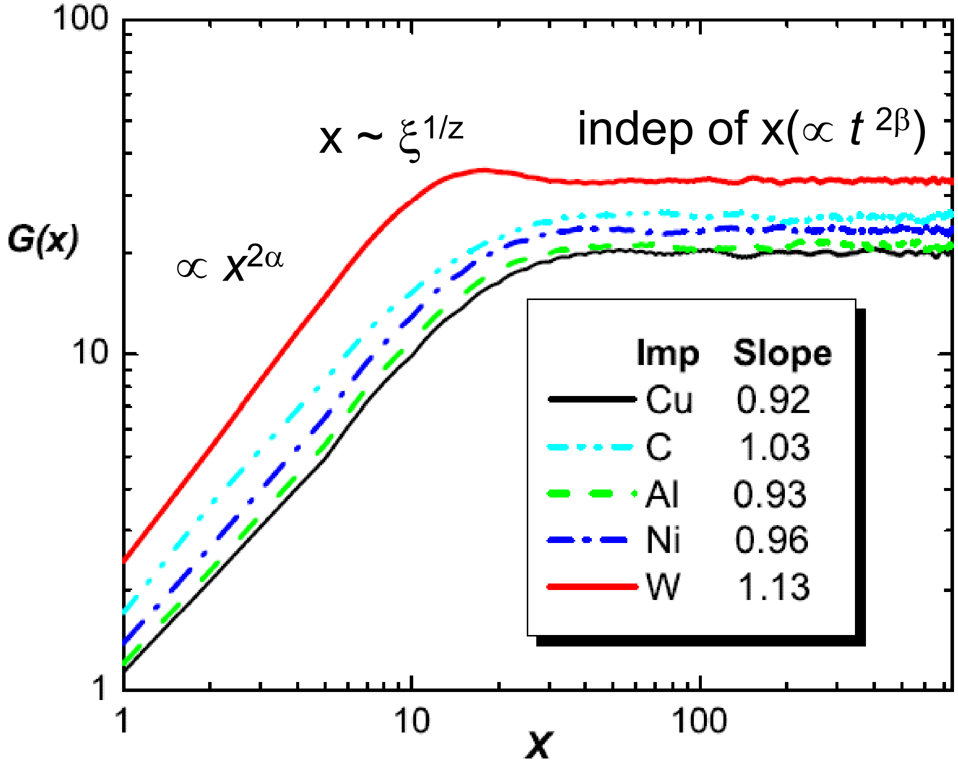
Sadly, apparatus no longer intact and available to examine

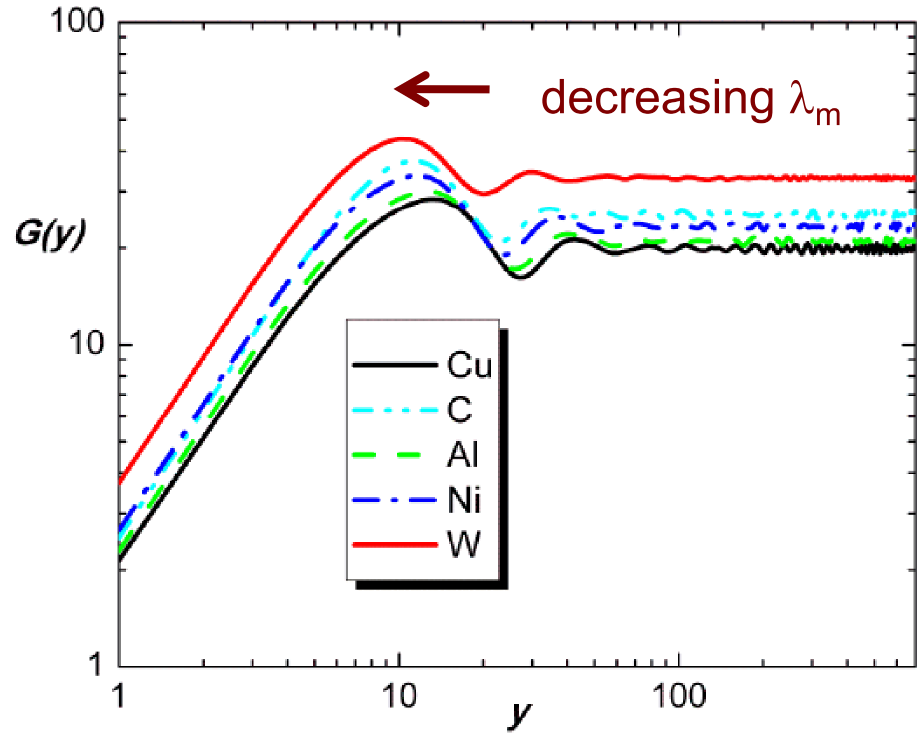
NB: Not S, since experimenters carefully desulfurized Cu. (T. Maroutian)

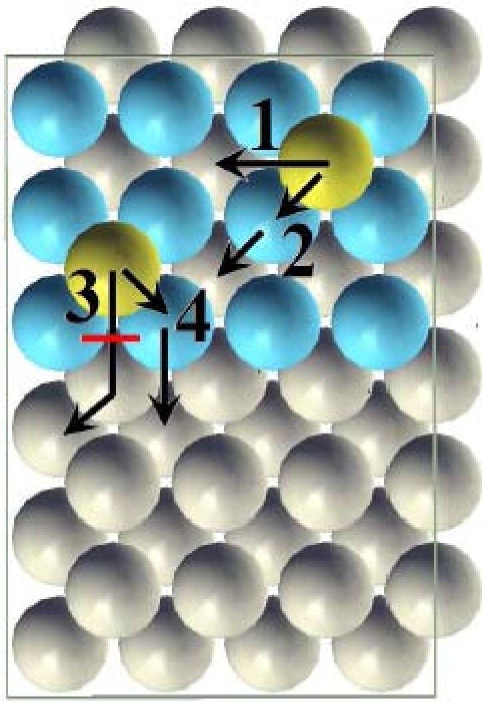
Height-height correlation functions



$$G(x,t) = \langle \overline{[h(\mathbf{r} + x\,\hat{\mathbf{e}}_x, t) - h(\mathbf{r}, t)]^2} \rangle$$







2) Embedding (emb), 3) hopping (hop), and 4) exchange (exc) diffusion barriers on Cu (001) computed with VASP

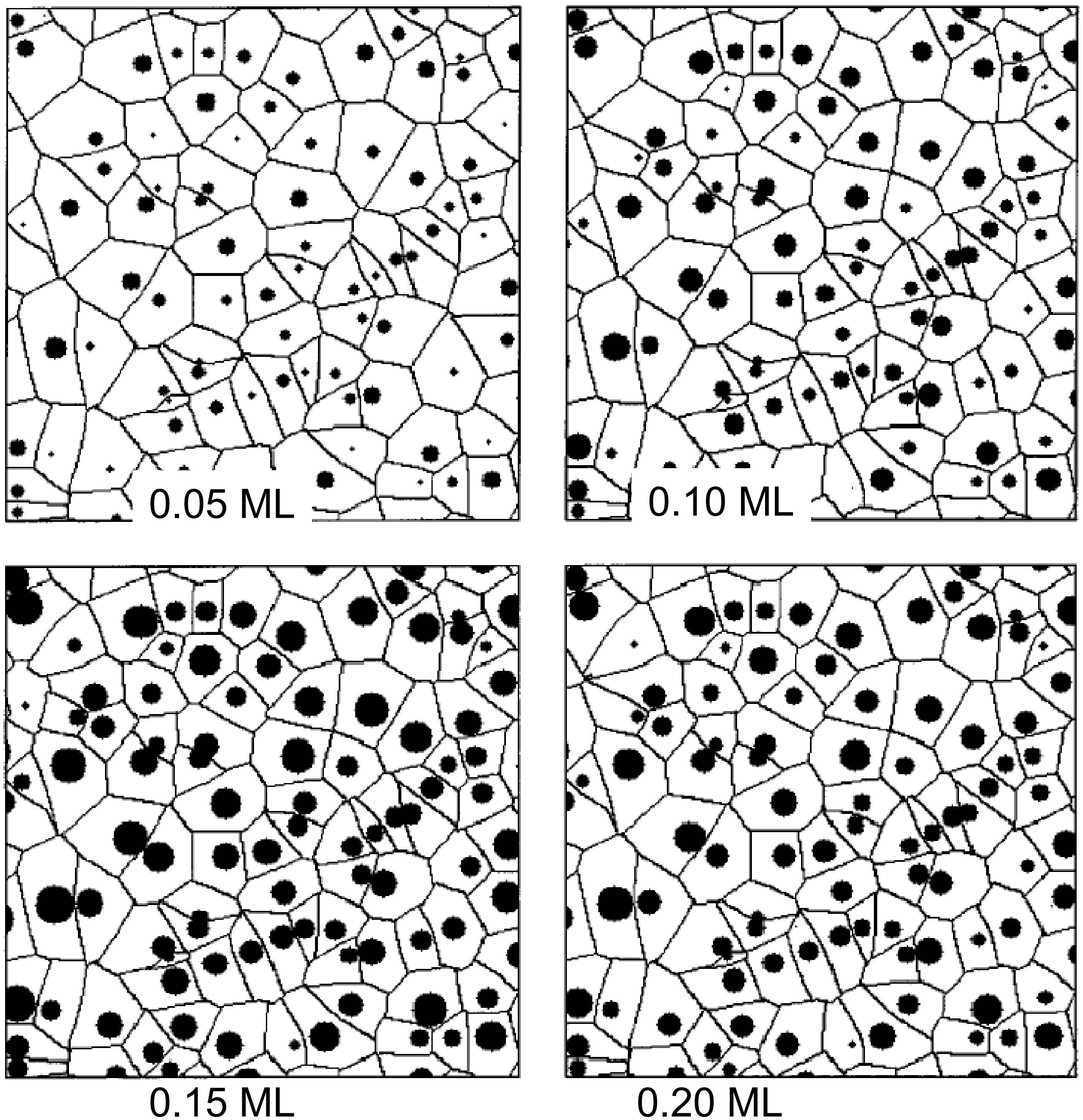
Very low E_{exc}. Cf. H. Yildirim and T. S. Rahman, Phys. Rev. B 80 ('09) 235413, not BAPS (Mar'09) Q12.07

Exchange moves not in our minimal model nor our algorithm

Quandary: reconcile meandering & small ES (E_{exc})

	1 E_d	2 E_{emb}	3 E_{hop} (E_{ES})	4 E_{exc}
Cu	0.550/0.0	0.695/0.0	0.695 (0.145)/0.408	0.510/0.408
Fe	0.911/0.0	0.427/0.756	1.316 (0.405)/0.544	0.295/0.980
Mn	0.865/0.0	0.397/0.863	1.334 (0.469)/0.613	0.233/1.088
W	0.880/0.0	0.262/1.690	1.845 (0.965)/0.882	0.094/1.767

Energies in eV   After /: E_{init} - E_{fin}



Evolution of Island Structures: Simulations of *Circular* Islands

Mulheran & Blackman, PRB 53 ('96) 10261

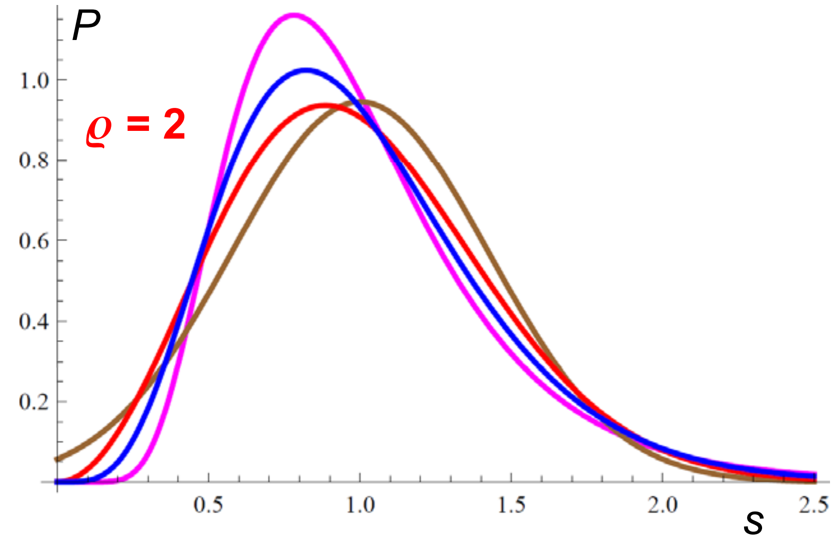
Can be more fruitful to study distribution of areas of *capture zones* (CZ) [Voronoi cells] than of island sizes!

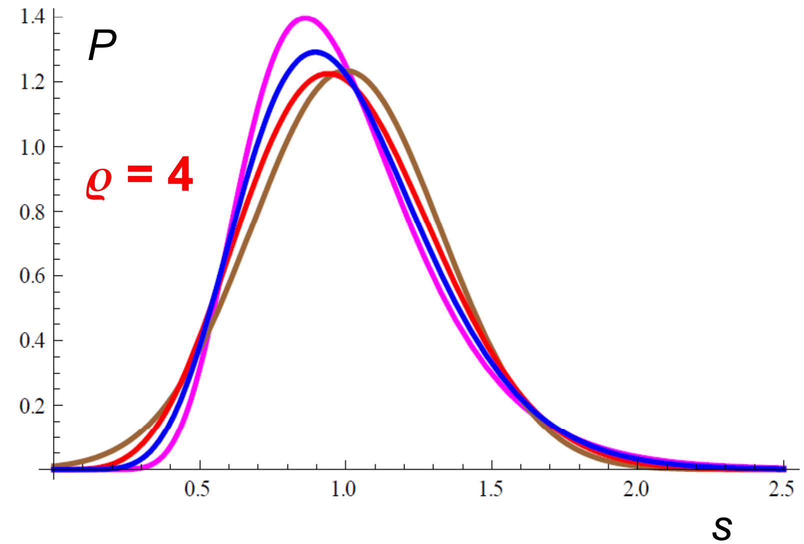
s = capture zone area/ average cap. zone area

Single-parameter distributions with mean = 1, same variance, in order of increasing skewness

- Gaussian: $P_\sigma(s) = (2\pi\sigma^2)^{-1/2} \exp[-(s-1)^2/2\sigma^2]$
  Mean-field-like; modest σ^2, significant probability for $s < 0$

- Generalized Wigner: $P_\varrho(s) = a_\varrho\, s^\varrho \exp(-b_\varrho s^2)$,
  var. = $[(\varrho+1)/2b_\varrho]-1$, $b_\varrho = [\Gamma(1+\varrho/2)/\Gamma(½+\varrho/2)]^2$
  Describes fluctuations of broad range of systems, inc. nuclear energy levels, chaotic orbits, based on symmetry for ϱ = 1,2,4 (orthogonal, unitary, or symplectic $\mathscr{H}$, via random matrix theory) generalizable to repelling fermions in 1D, terrace-width distributions on vicinal surfaces (with related to strength of dimensionless ℓ^{-2} elastic repulsion between steps, etc.





- Gamma: $P_\varrho(s) = [\alpha^\alpha/\Gamma(\alpha)]\, s^{\alpha-1} \exp(-\alpha s)$, var. = α^{-1}

Exact for random point deposition in 1D [Kiang, Z. Astrophys. 64 ('66) 433], but does not generalize to larger islands or higher D; used for foams & froths by Weaire et al.

- Log-normal: $P_\sigma(s) = (2\pi\sigma^2)^{-1/2}\, s^{-1} \exp[-(\ln(s)+\sigma^2/2)^2/2\sigma^2]$,
  var. = $\exp(\sigma^2)-1$,
  product of many indep. positive random variables

$b \approx i + 2$
$= i + 1$ in mean field

Calogero-Sutherland Model's Ground State & Random Matrices

Calogero-like Hamiltonian:

$$\mathcal{H} = -\sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} + 2\frac{\beta}{2}\left(\frac{\beta}{2} - 1\right) \sum_{1\le i<j\le N} (x_j - x_i)^{-2} + \omega^2 \sum_{j=1}^{N} x_j^2$$

Positions of fermions (steps) ↔ eigenenergies of nuclei, for Hamiltonians with orthogonal, unitary, or symplectic symmetry! So step spacings (s) ↔ energy spacings. *Miraculously*, $|\Psi_0|^2$ of C-S models corresponds to exact $P(s)$ of RMT for cases ϱ = 1, 2, & 4. But $\varrho = 1 + (1+4Ã)^{1/2}$ need not have these values. $P_\varrho(s)$ is a good approx. of exact P for these 3 values so why not for all $\varrho > 0$?!

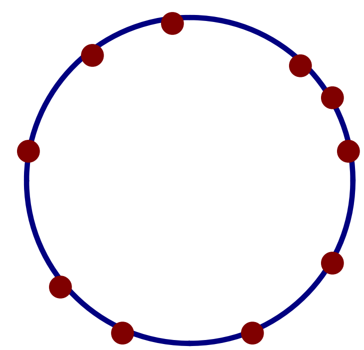
… $\to \infty$, $\omega \to 0$; in Calogero $\mathcal{H}$, $x_j^2 \to (x_j - x_i)^2$.]

$$\Psi_0 = \prod_{1\le i<j\le N} |x_j - x_i|^{\varrho/2} \exp\left(-\frac{1}{2}\omega \sum_{k=1}^{N} x_k^2\right)$$

…l-state density Ψ_0^2 is recognized as a joint probability distri-
…n from the theory of random matrices for Dyson's Gaussian

…Hamiltonian:

$$\ldots -\sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} + 2\frac{\beta}{2}\left(\frac{\beta}{2} - 1\right) \frac{\pi^2}{L^2} \sum_{i<j} \left[\sin\frac{\pi(x_j - x_i)}{L}\right]^{-2}$$



$$\Psi_0 = \prod_{i<j} \left|\sin\frac{\pi(x_j - x_i)}{L}\right|^{\varrho/2}, \quad x_j > x_i$$

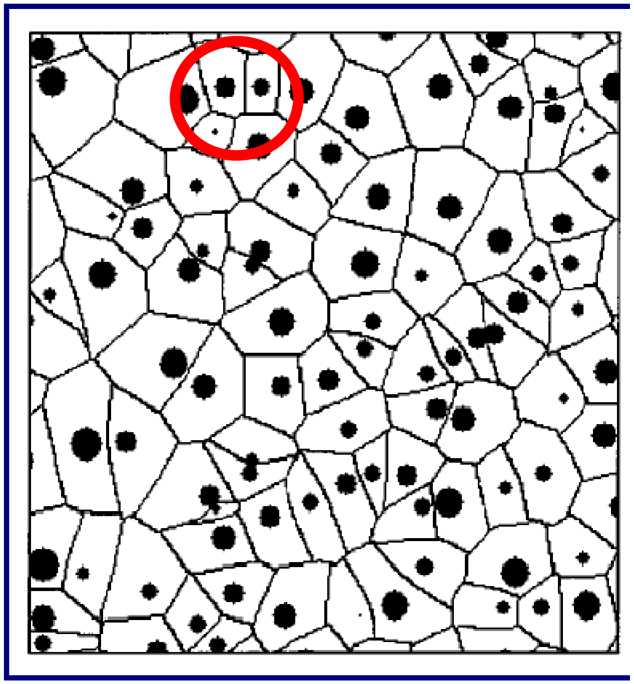
$$\theta_i \equiv 2\pi x_i / L \quad \Rightarrow \quad \Psi_0^2 = \prod_{i<j} \left|e^{i\theta_j} - e^{i\theta_i}\right|^{\varrho}$$

…l-state density Ψ_0^2 is also a joint probability distribution func-
…heory of random matrices, now for Dyson's circular ensembles.
…he pair correlation functions and other properties of the ensem-
…luated exactly only for the cases $\beta = 1$, 2, or 4, corresponding
to orthogonal, unitary, or symplectic symmetry of the ensemble.

Phenomenological mean-field theory

CZ does "random walk" with 2 competing effects on *ds/dt*:

1] Neighboring CZs hinder growth ⇒ external pressure
leads to force opposing large *s*
Also noise since atom can go to "wrong" island



2] Non-symmetric confining potential, newly nucleated island has non-tiny CZ, comparable to neighbors so force stops fluctuations of CZ to tiny values

3] Nucleation rate
$\propto$ adatom density x density of critical nuclei
$\propto$ (adatom density)$^{(i+1)}$ [Walton relation]

4] New CZ in region of very small CZs will have size comparable to those nearby, so very small also

5] Combine to Langevin eq. $ds/dt = K\,[(i+1)/s - Bs] + \eta$
Leads to Fokker-Planck eq. with stationary sol'n $P_\varrho(s)$
cf. AP, HG, & TLE, Phys. Rev. Lett. **95** ('05) 246101

Comparison with refined simulations for *compact* islands: $\varrho \approx i+2^{-}$

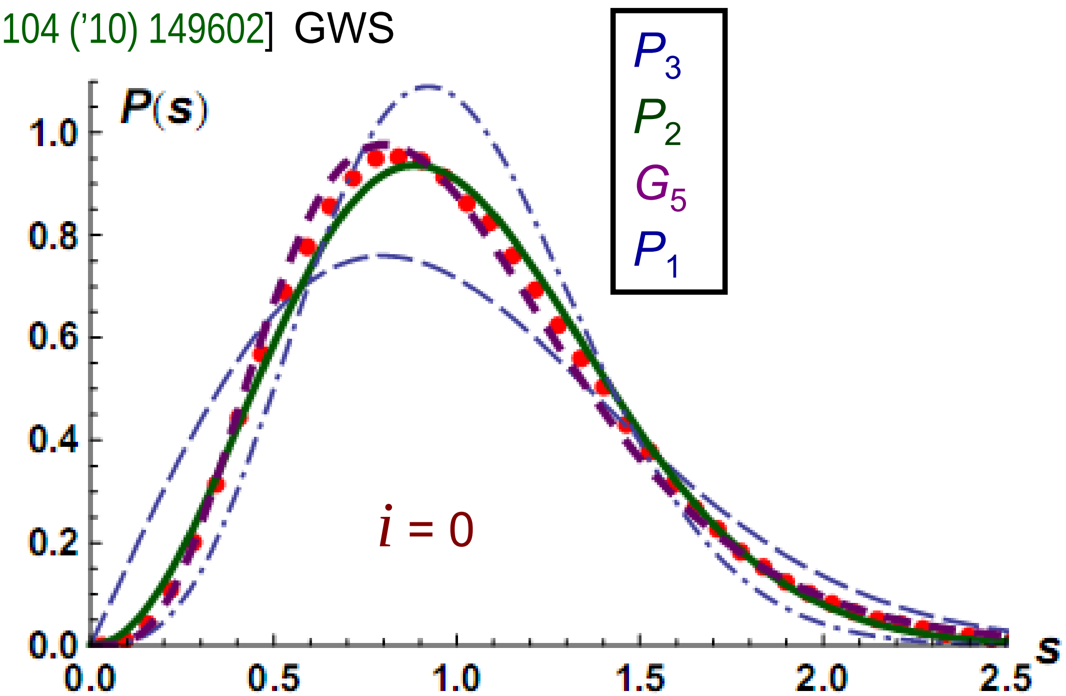
Mean field argument [AP& TLE, PRL 99 ('07) 226102] predicted $\varrho = i + 1$

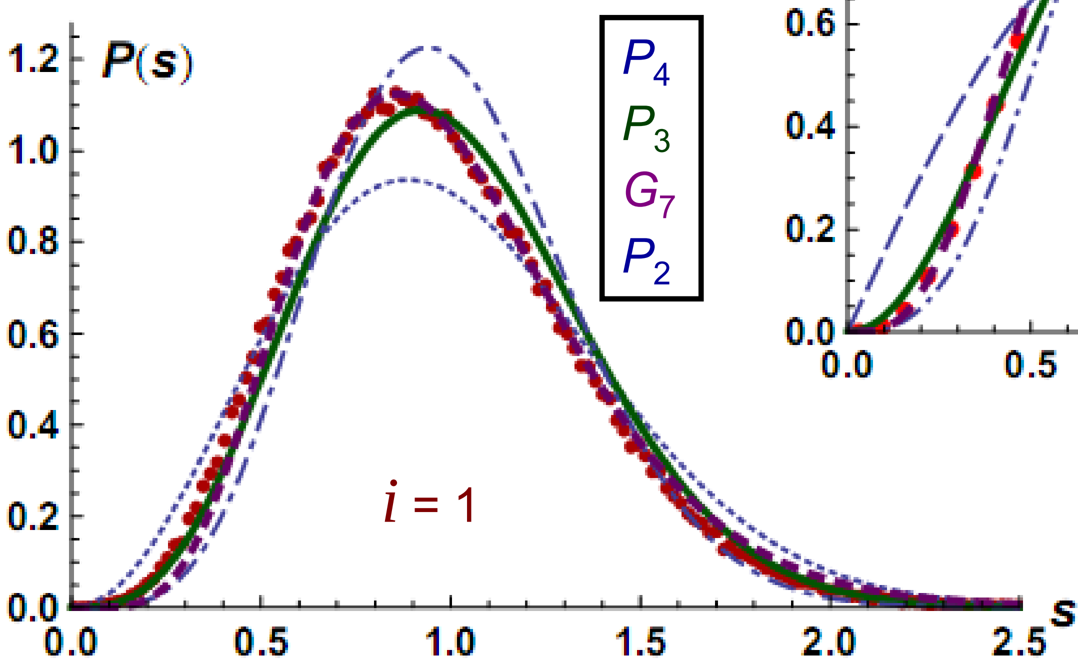
- ● numerical data [Li, Han, Evans, PRL Comment 104 ('10) 149601 & pvt.; points islands–Shi, Shim, Amar, PRE 79 ('09) 011602]

— $P_{i+2}(s)$ [Pimpinelli & Einstein, PRL Reply 104 ('10) 149602] GWS

— - - $P_{i+2\pm1}(s)$

– – $G_{2i+5}(s)$ gamma distribution





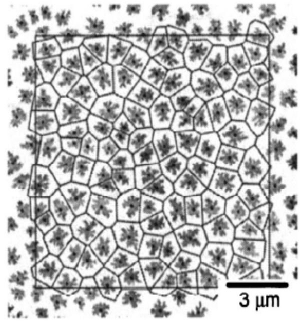
Best fit of extensive data: between $P_{i+2}(s)$ & $G_{2i+5}(s)$

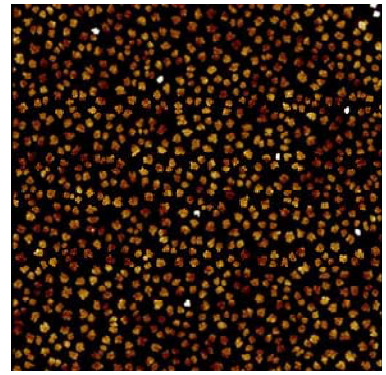
Fractal/ramified islands not yet scrutinized

View i as an effective parameter

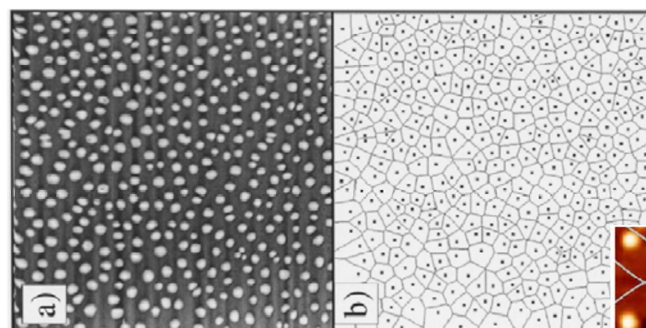
Applications to actual (not MC) experiments

- Pentacene/SiO_2

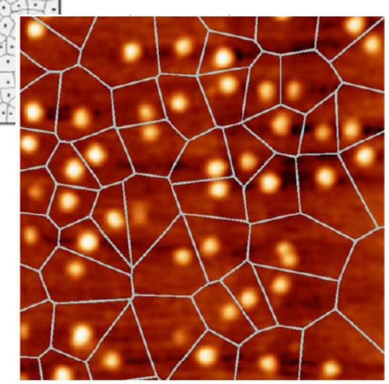




- Pentacene-PentaceneQuinone

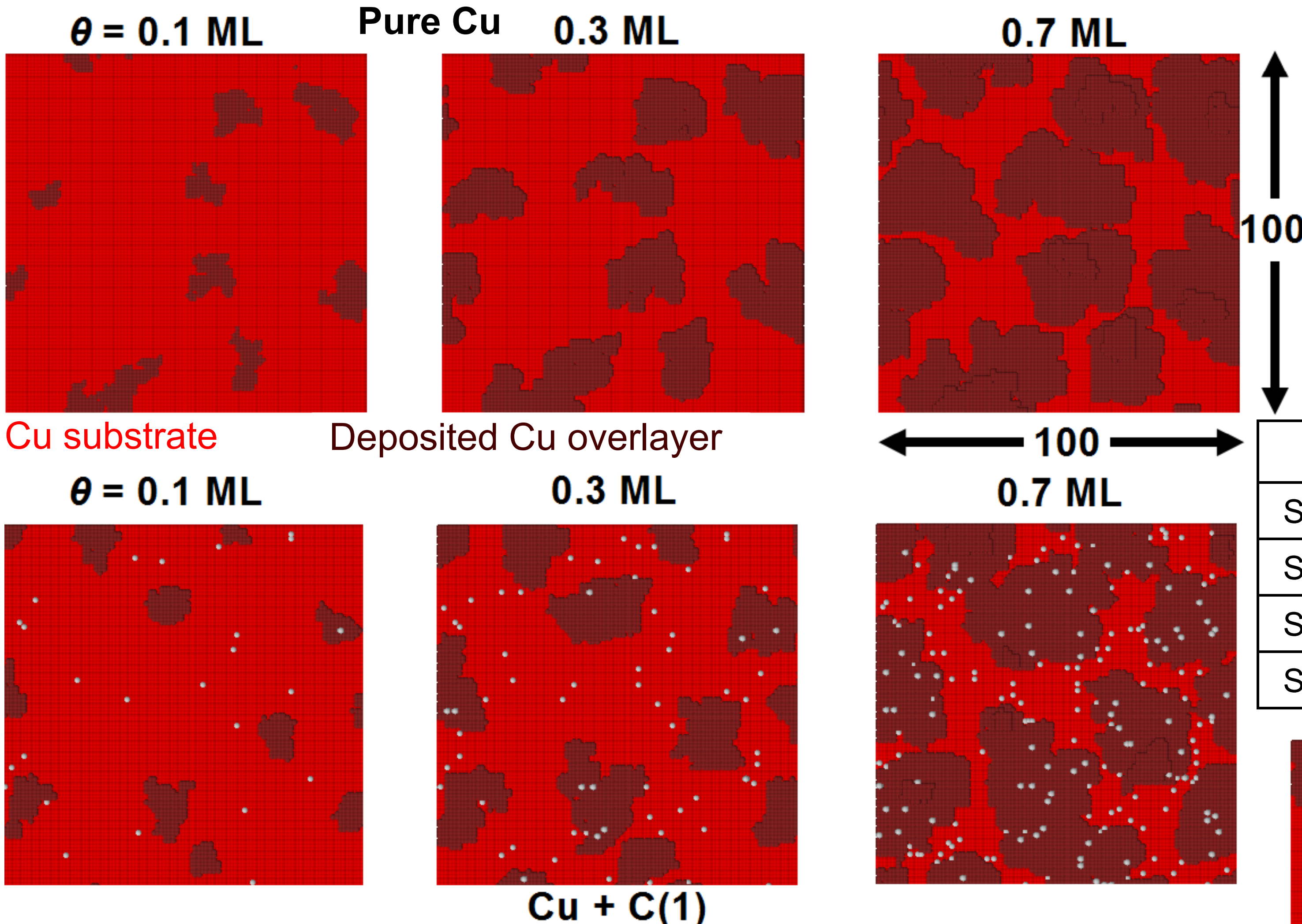


- Alq_3 on passivated Si(100)



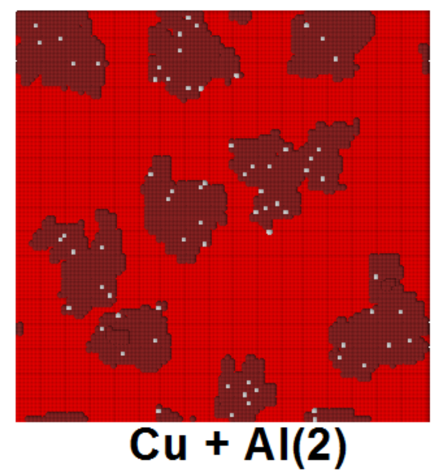
- InAs *quantum dots* on GaAs(001)

Growth-morphology differences are already visible at submonolayer coverage-1



Lattice = 800×800
***T* = 425 K,**
***F* = 5×10^{-2} ML/s**
Impurity Conc: **2%**

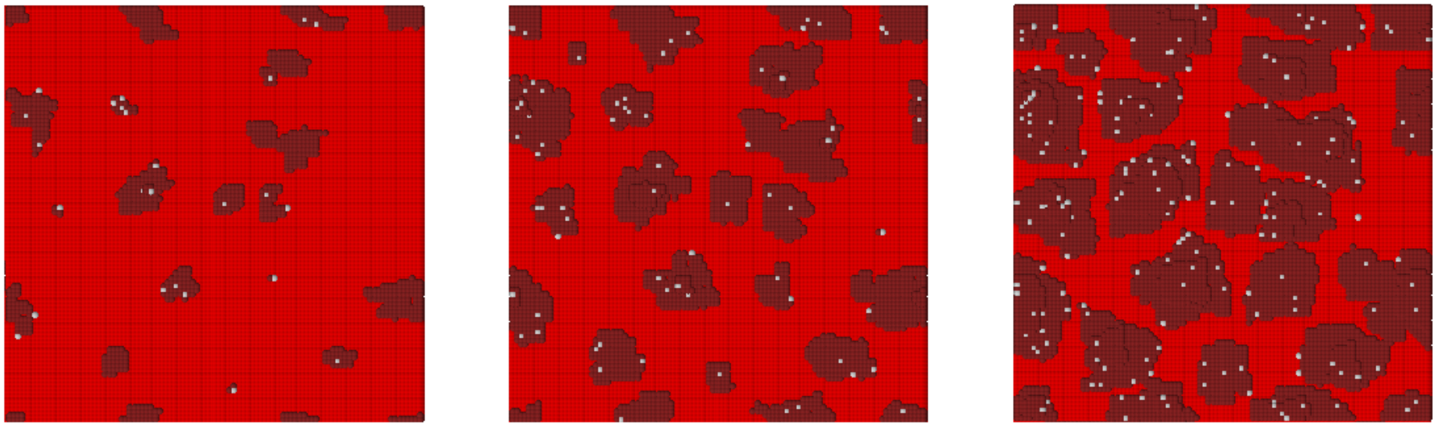
Impurity sets	
Set 1	**O, C, S**
Set 2	**Ag, Sn, Zn, Al**
Set 3	**Pd, Ni, Si**
Set 4	**Co, Fe, Mn, W**



- Pure Cu: nr. islands (N_i) does not change with coverage
- Cu with C: single impurity atoms + large islands
- Cu with Al: very similar to pure Cu

Growth-morphology differences are already visible at submonolayer coverage-2

θ = 0.1 ML | **0.3 ML** | **0.7 ML**

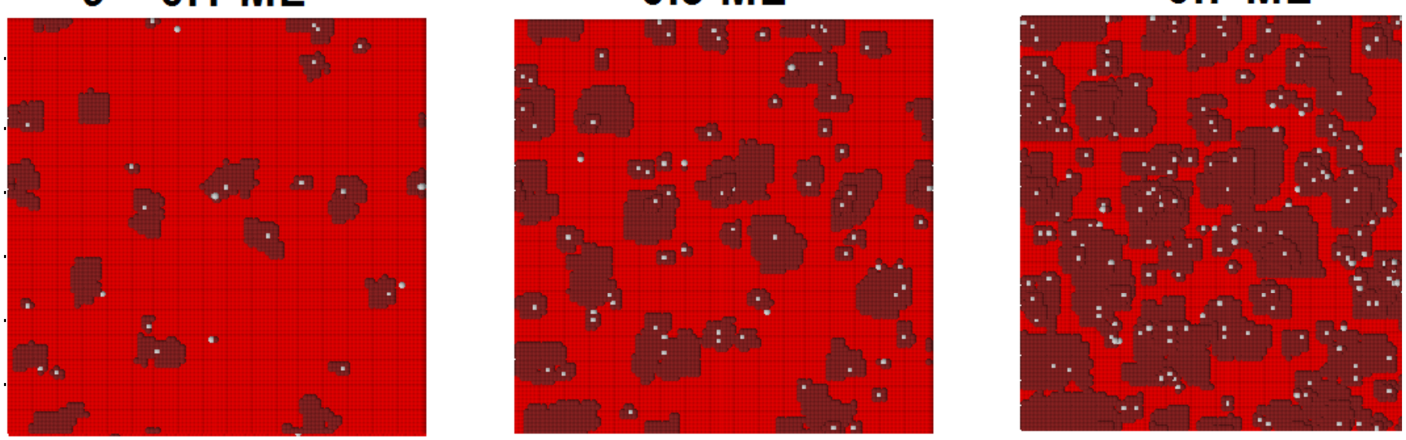


Cu + Ni(3)

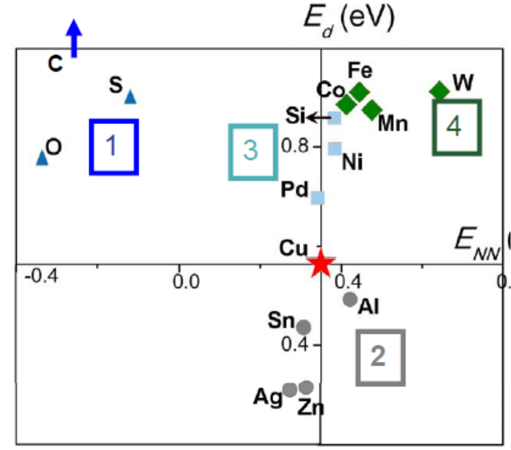
Lattice = 800×800
***T* = 425 K,**
***F* = 5×10^{-2} ML/s**
Impurity Conc. = 2%

- Cu with Ni: small islands, nr. of islands (N_i) increases with coverage (θ)
- Cu with W: similar to Ni but more small islands

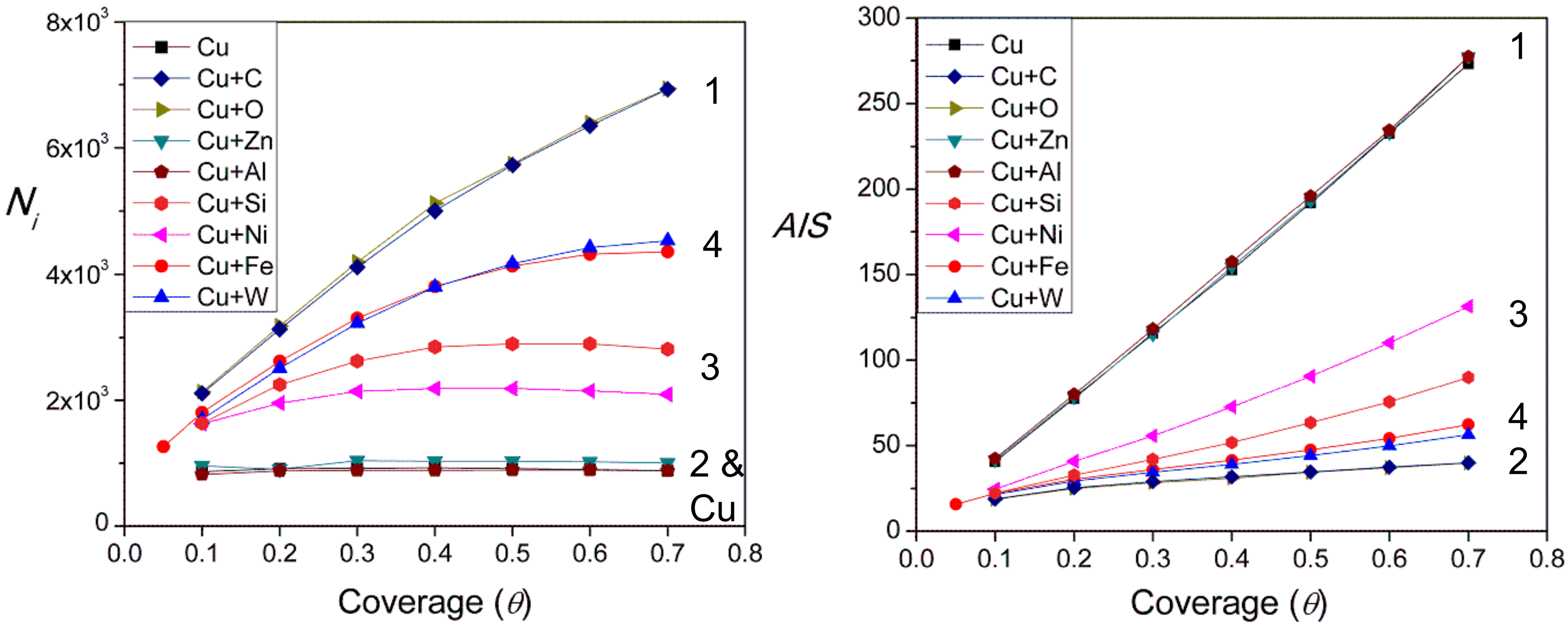
θ = 0.1 ML | **0.3 ML** | **0.7 ML**



Cu + W(4)



How do impurities affect island nucleation?

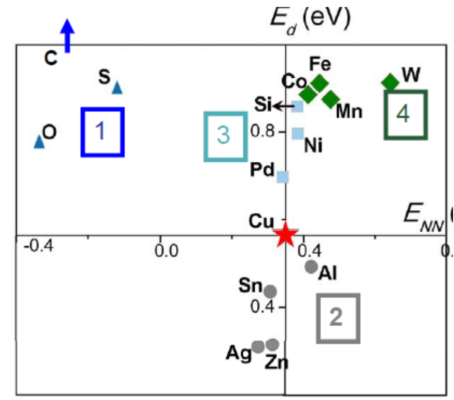


- Number of islands (N_i): rapid increase ⟶ slow increase ⟶ decrease (coalescence)
- Average island size (*AIS*) increases with θ throughout the regime for all impurities

Codeposition of impurities from different (same) sets leads to significantly different (similar) island nucleation and growth behavior in the sub-monolayer regime.

Impurity sets	
Set 1	**O, C, S**
Set 2	**Ag, Sn, Zn, Al**
Set 3	**Pd, Ni, Si**
Set 4	**Co, Fe, Mn, W**

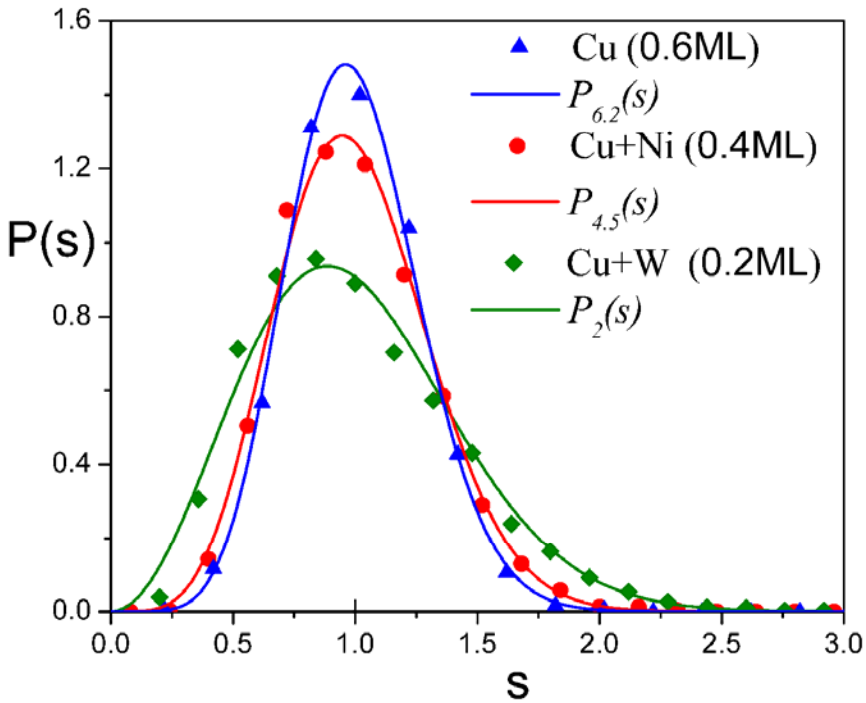
Distribution of Capture-zone Areas

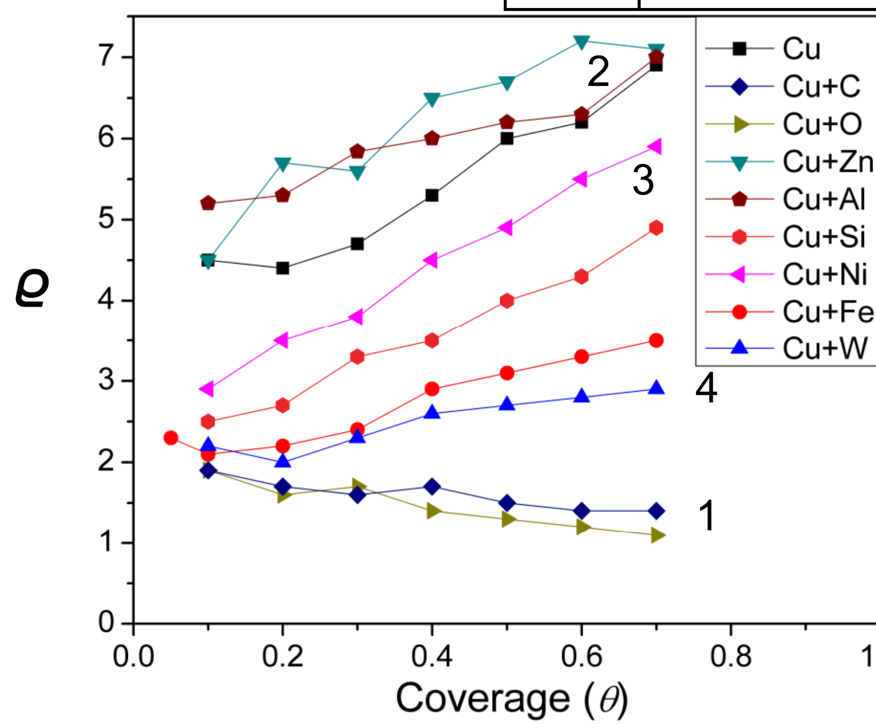


- GWD gives good fits to CZ-area distribution in the presence of different impurities (NB: extension from standard single-species)
- ϱ increases with θ for all cases except Cu with set-1 impurities – due to repulsive E_{NN}, single impurity atom islands?
- In general, higher E_d and higher E_{NN} values lead to smaller ϱ, due to reduction in the critical cluster size (i)

Impurity sets	
Set 1	**O, C, S**
Set 2	**Ag, Sn, Zn, Al**
Set 3	**Pd, Ni, Si**
Set 4	**Co, Fe, Mn, W**

$$P_{\varrho}(s) = as^{\varrho}e^{-bs^2}$$





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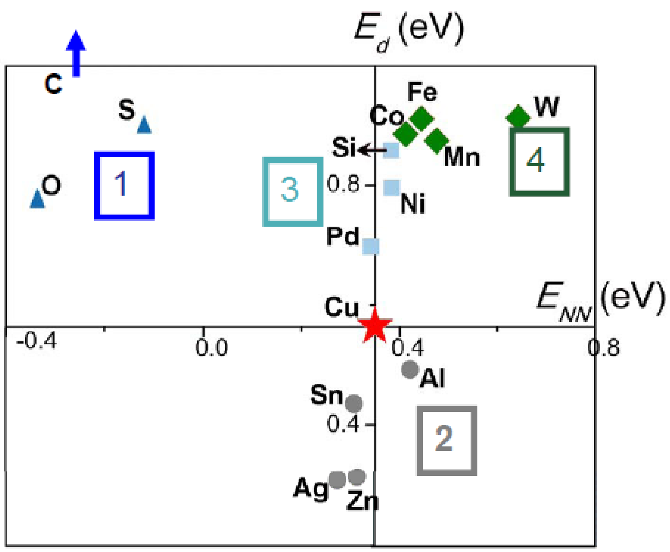
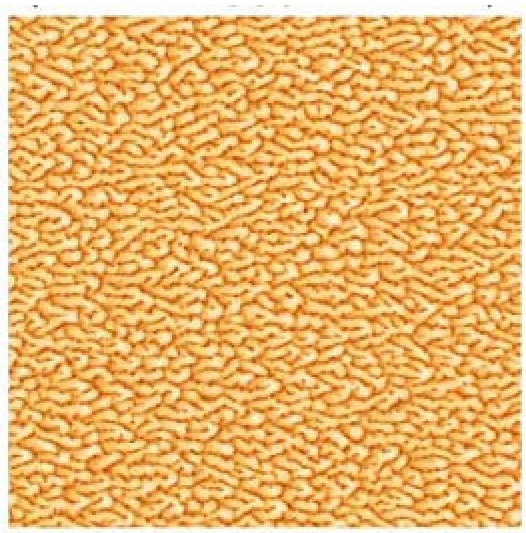
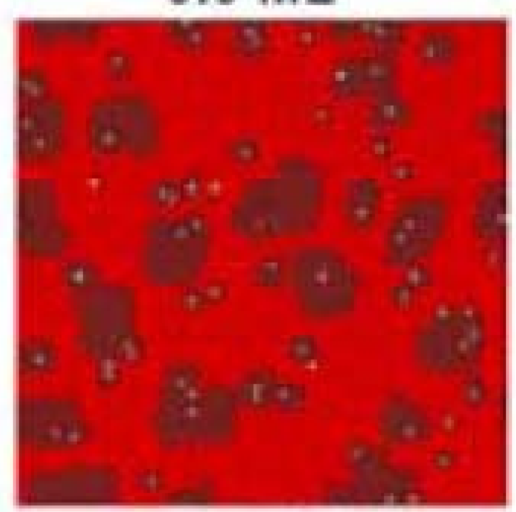
Role of Codeposited Impurities During Growth: I. Explaining Distinctive Experimental Morphology on Cu(0 0 1), Ajmi BH. Hamouda, Rajesh Sathiyanarayanan, A. Pimpinelli, and TLE, submitted to PRB.

Role of Codeposited Impurities During Growth: II. Dependence of Morphology on Binding and Barrier Energies, Rajesh Sathiyanarayanan, Ajmi BH. Hamouda, A. Pimpinelli, and TLE, submitted to PRB

CZD & Wigner, AP & TLE, Phys. Rev. Lett. 99 ('07) 226102 ; 104 ('10) 149602 (& 149601)




(d) Cu+W

0.3 ML

Cu + W(4)

Conclusions - 1

kMC study of the effect of impurities on vicinal-surface step-flow growth
→ Agreement with Cu exp't: morphology & $\lambda(F)$.

- **Comparison** with exp't on vicinal Cu supports the hypothesis that many previously unexplained features of the meandering instability are due to impurities.
- **Impurities:** responsible for *qualitative* & *quantitative* modification of the surface morphology:
  - ***nucleation centers*** → *pyramids*
  - ***diffusion less dependent on F*** → *wavelength*
- **DFT (VASP) study** : *impurity & concentration*
  Mid-transition (Fe, Mn, W) rather than gases
- Experimental apparatus info strongly suggests that W is the culprit

Conclusions - 2

- Based on their E_{NN} and E_d values (relative to the values for Cu), impurity atoms can be classified into sets
- Our simulations show that codeposition of impurities from different sets with Cu result in siginificantly different surface morphologies for growth:
  - in the step-flow mode (θ = 40 ML) and
  - in the submonolayer regime ($\theta \leq$ 0.7ML)
- Generalized Wigner distribution fits well the distribution of capture-zone areas for pure Cu and Cu codeposited with impurities. However, the exact connection between the fit parameter ϱ and i is not clearly known.
- Growth morphologies can be controlled through the codeposition of appropriate impurity atoms.
- Dramatic effect of impurities on growth → *self-nanostructuring / stabilizing*

(Let's Get) Physical
Olivia Newton-John

I'm saying all the things that I know you'll like,
Makin' good conversation
I gotta handle you just right,
You know what I mean
I took you to an intimate restaurant,
Then to a suggestive movie
There's nothin' left to talk about,
Unless it's horizontally

Let's get physical, physical,
I wanna get physical, let's get into physical
Let me hear your body talk,
Your body talk, let me hear your body talk

I've been patient, I've been good,
Tried to keep my hands on the table
It's gettin' hard this holdin' back,
You know what I mean
I'm sure you'll understand my point of view,
We know each other mentally
You gotta know that you're bringin' out
The animal in me

Let's get animal, animal,
I wanna get animal, let's get into animal
Let me hear your body talk,
Your body talk, let me hear your body talk.