Emerging surface roughness during plastic deformation

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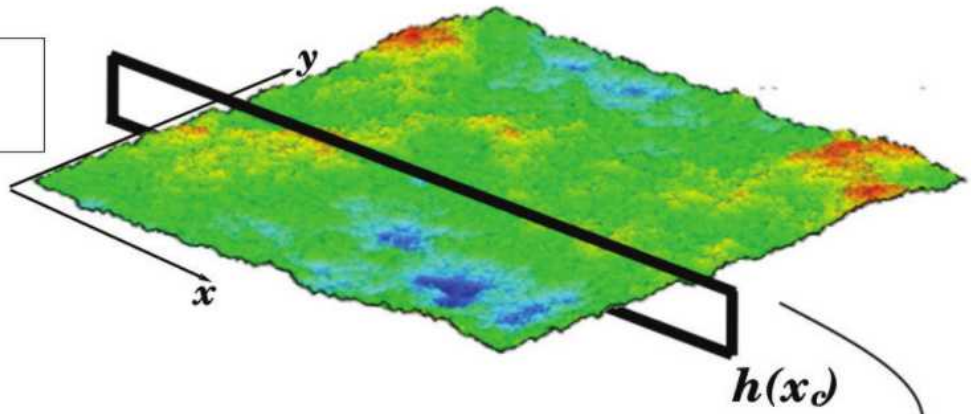
CECAM Workshop

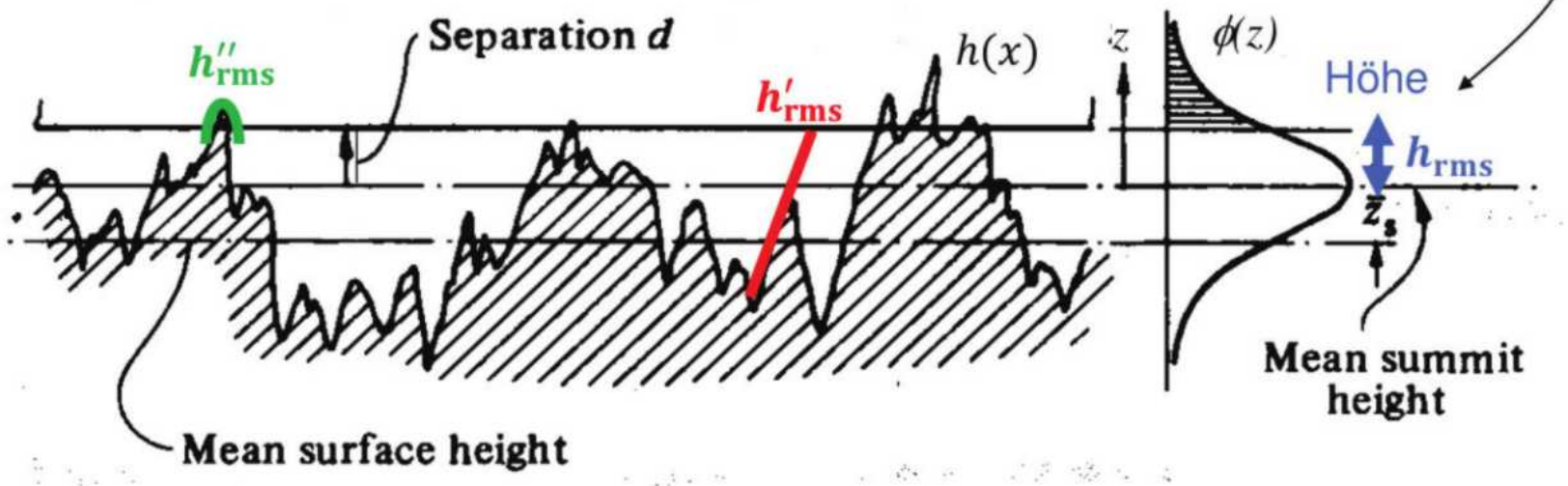
Emergence of surface and interface structure from friction, fracture and deformation

Lausanne, Switzerland
July 2018

Surface topography and roughness

Height Profile $h(x,y)$





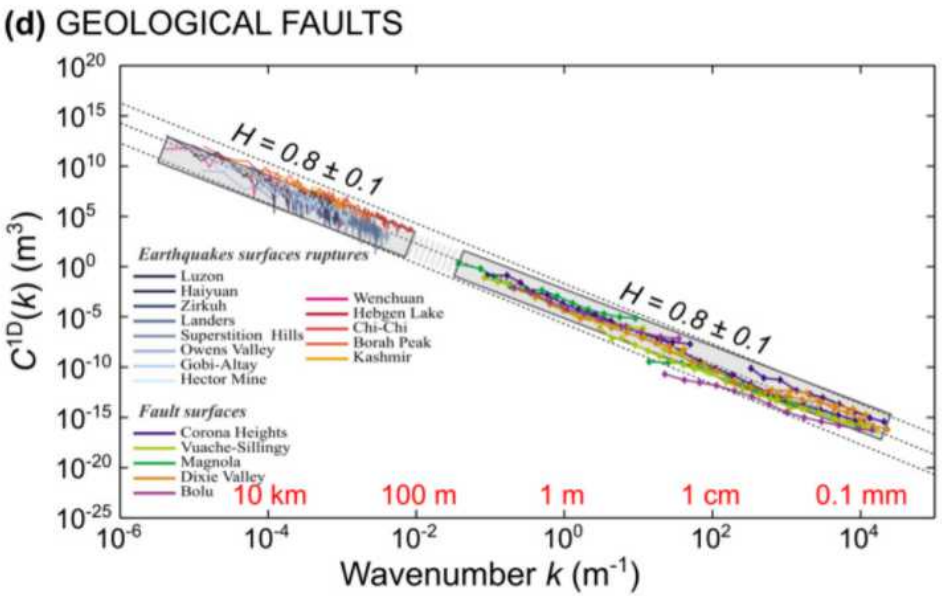
$$h''_{rms} = \frac{1}{2}\sqrt{\langle(\nabla^2 h)^2\rangle} \qquad h'_{rms} = \sqrt{\langle|\nabla h|^2\rangle} \qquad h_{rms} = \sqrt{\langle h^2\rangle}$$

Greenwood, Williamson, *Proc. Roy. Soc. Lond. A* 295, 300 (1966)

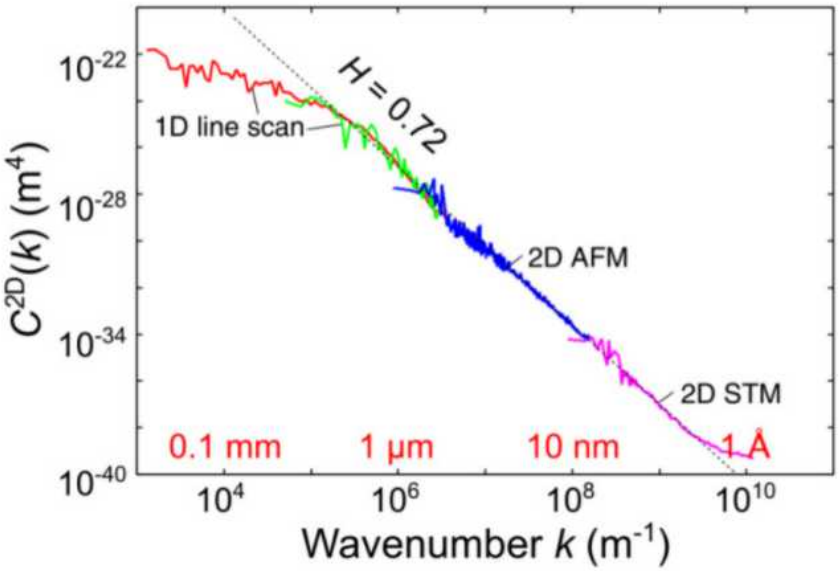
Self-affine system

$$C(\boldsymbol{q}) = \frac{1}{(2\pi)^2} \int d^2x \ \langle h(\boldsymbol{x}), h(\boldsymbol{x} + \delta\boldsymbol{x}) \rangle e^{-i\boldsymbol{x}\cdot\boldsymbol{q}}$$

$C(q) \sim q^{-2(1+H)}$ where H ranges from 0 - 1



T. Candela et al., J. Geophys. Res. Solid Earth 117, 1 (2012)

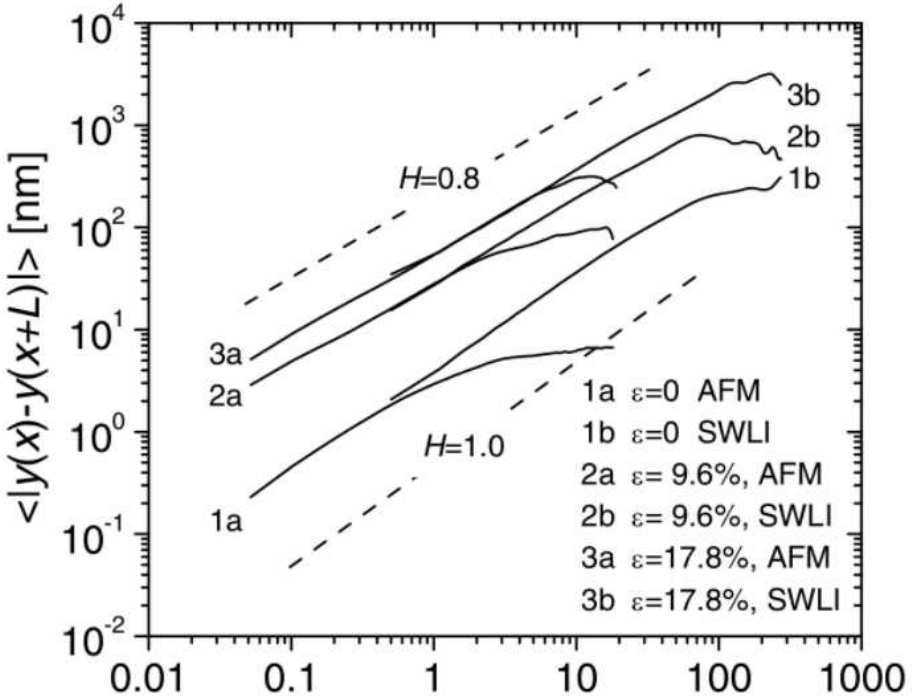


B.N.J. Persson, Tribol. Lett. 54, 99 (2014)

A common origin in plastic deformation? Quantify?

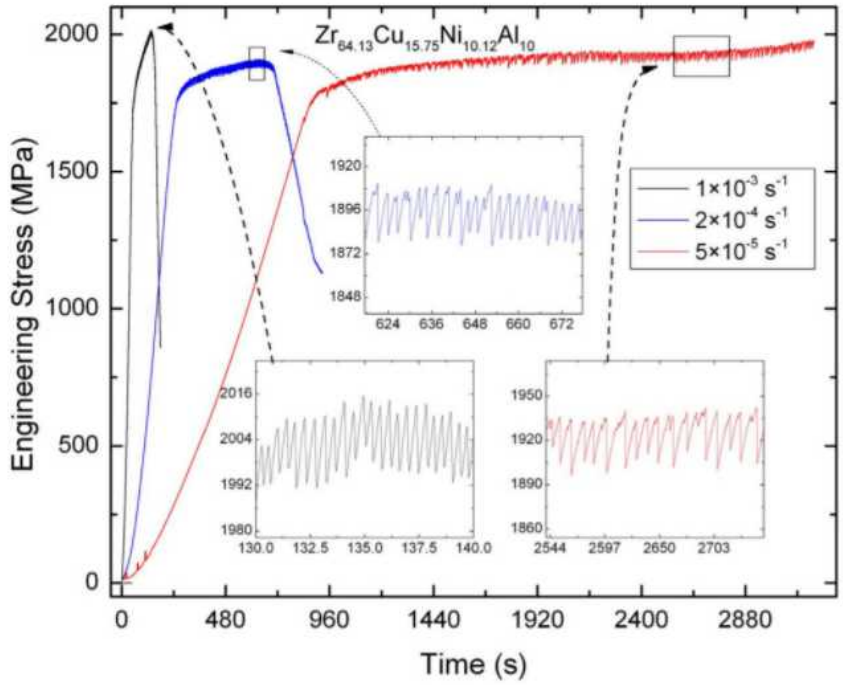
Plasticity and self-affine scaling

Experiments of polycrystalline Cu and single–crystal KCl



M. Zaiser et al. Phy. Rev. Lett. 93 (2004)
J. Schwerdtfeger et al., J. Stat. Mech. (2007) L04001

Experiments of metallic glasses



Antonaglia, J. et. al. Sci. Rep. 4, 4382(2014)

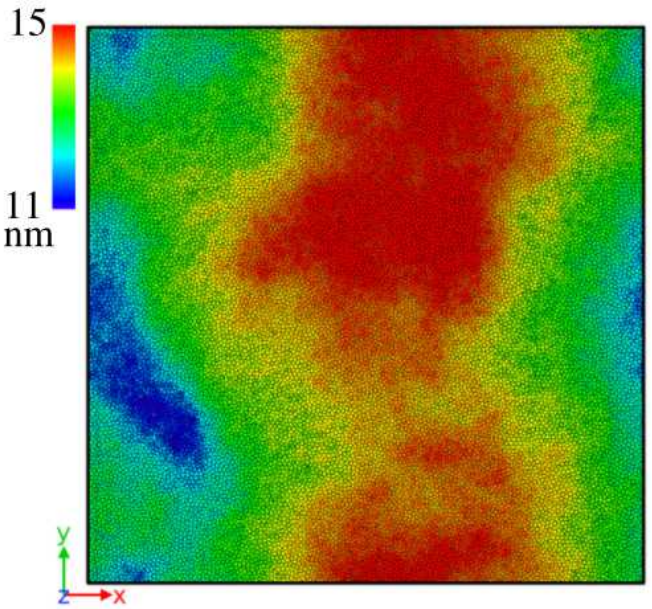
1D ONLY

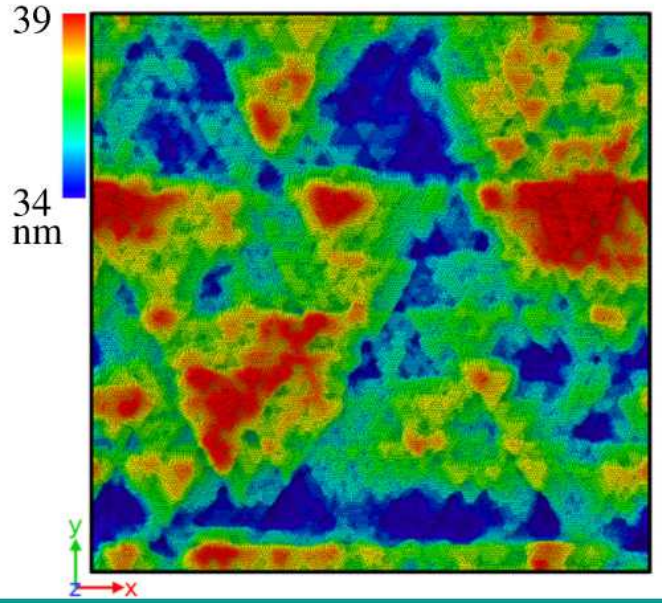
NO ATOMISTIC STUDIES

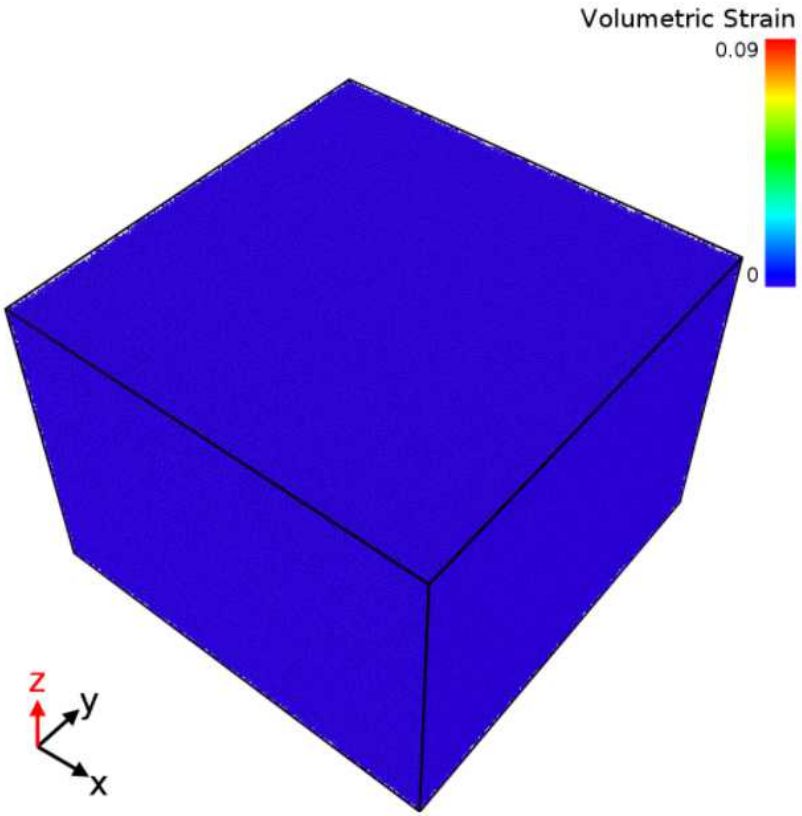
NO ATOMISTICS OF ROUGHNESS & SELF AFF.

NO EXPERIMENTS OF ROUGHNESS & SELF AFF.

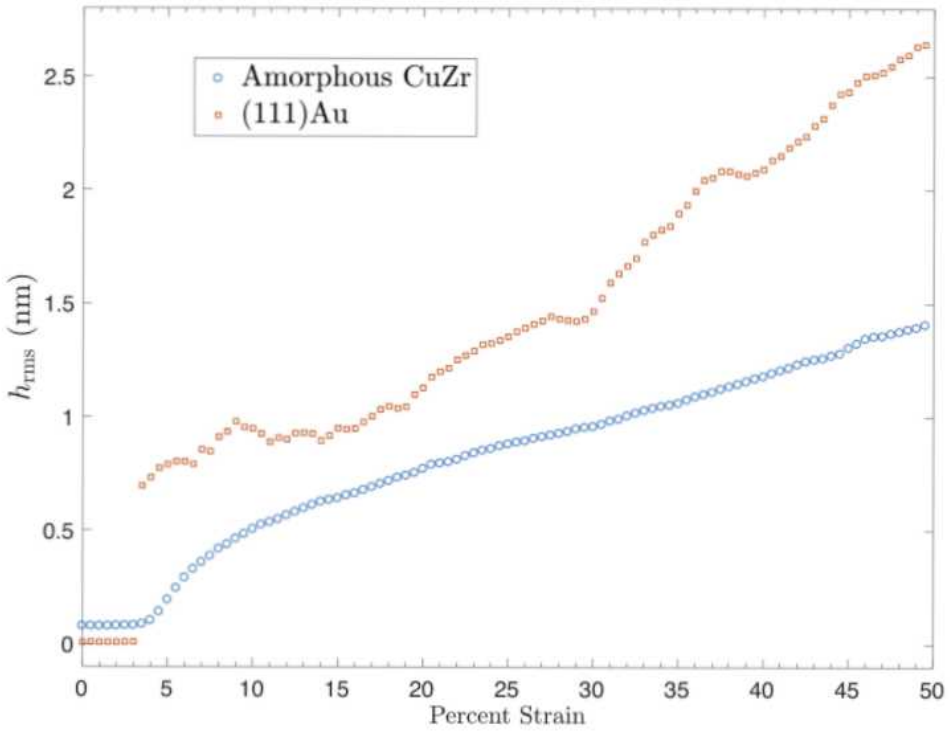
Bi-axial compression of amorphous CuZr and Au(111)

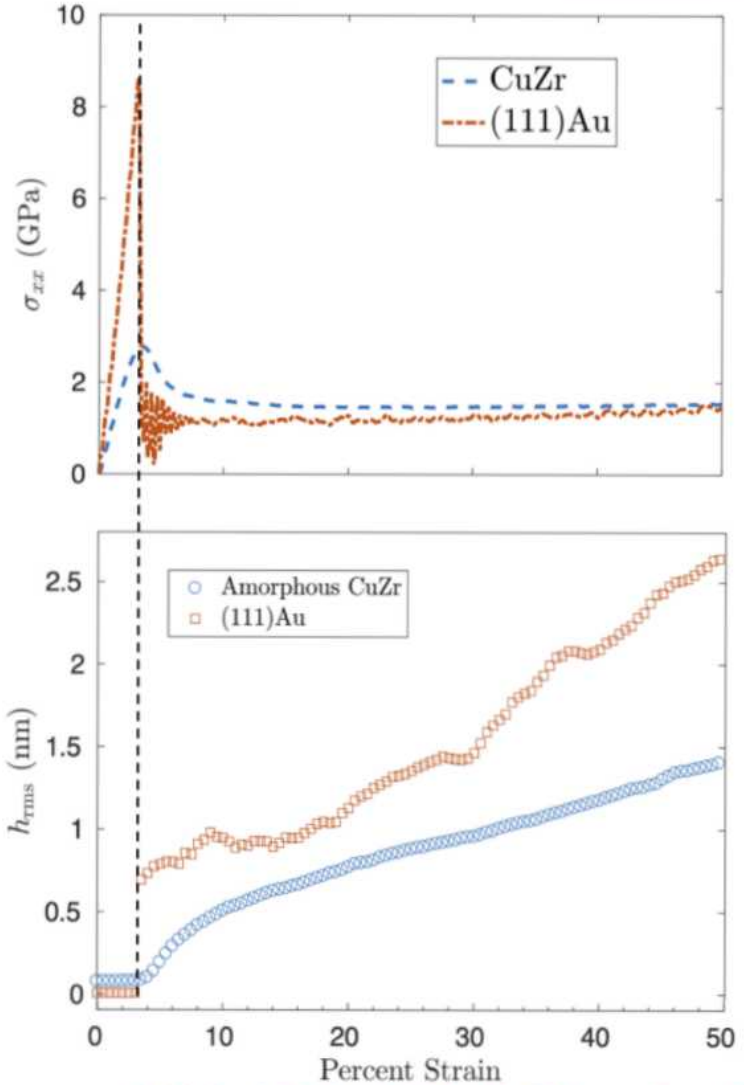


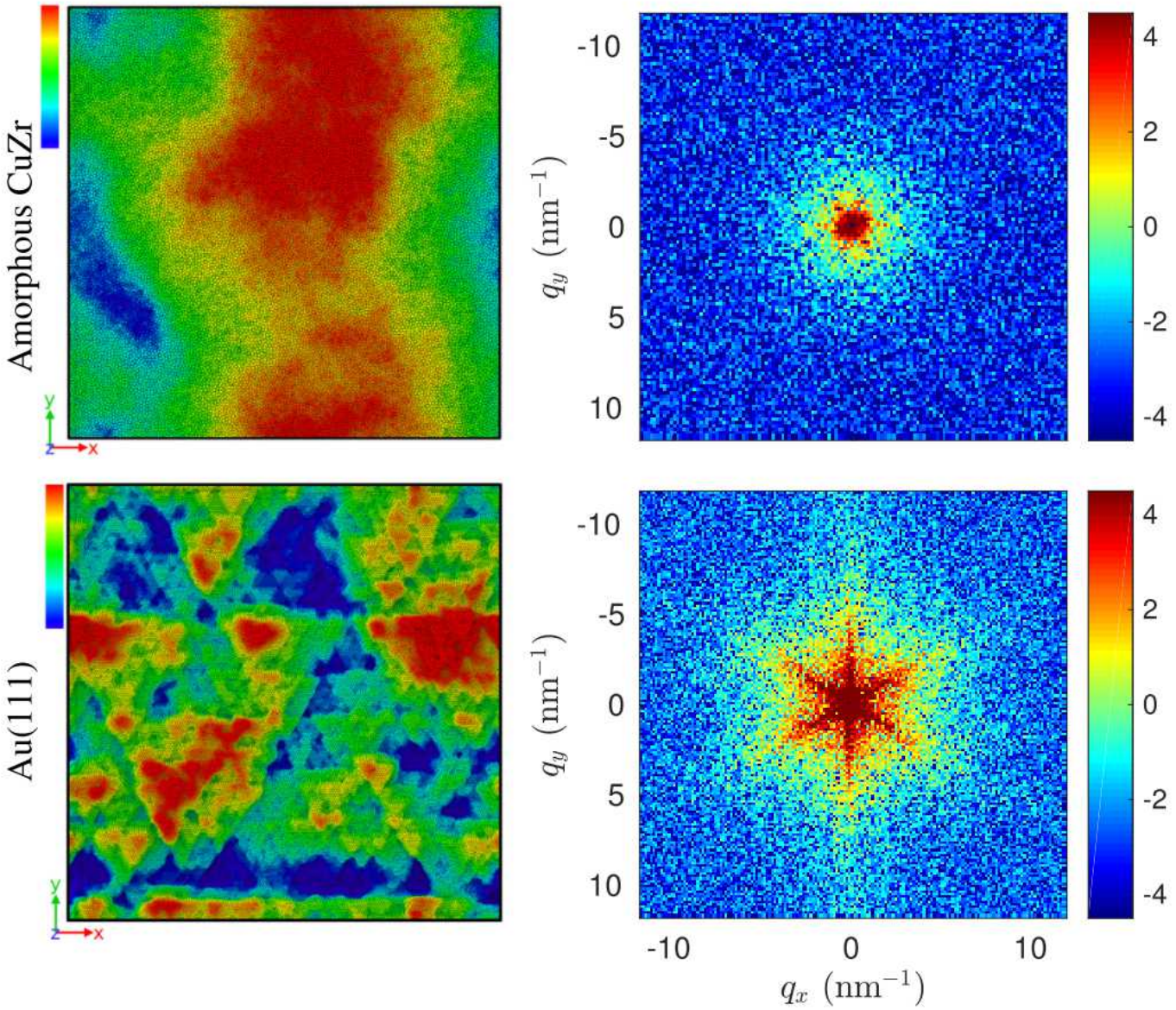




$$h_{\text{rms}} = \sqrt{\frac{1}{nm}\sum_{i=1}^{n}\sum_{j=1}^{m}\left(z(x_i, y_j) - \mu\right)^2}$$

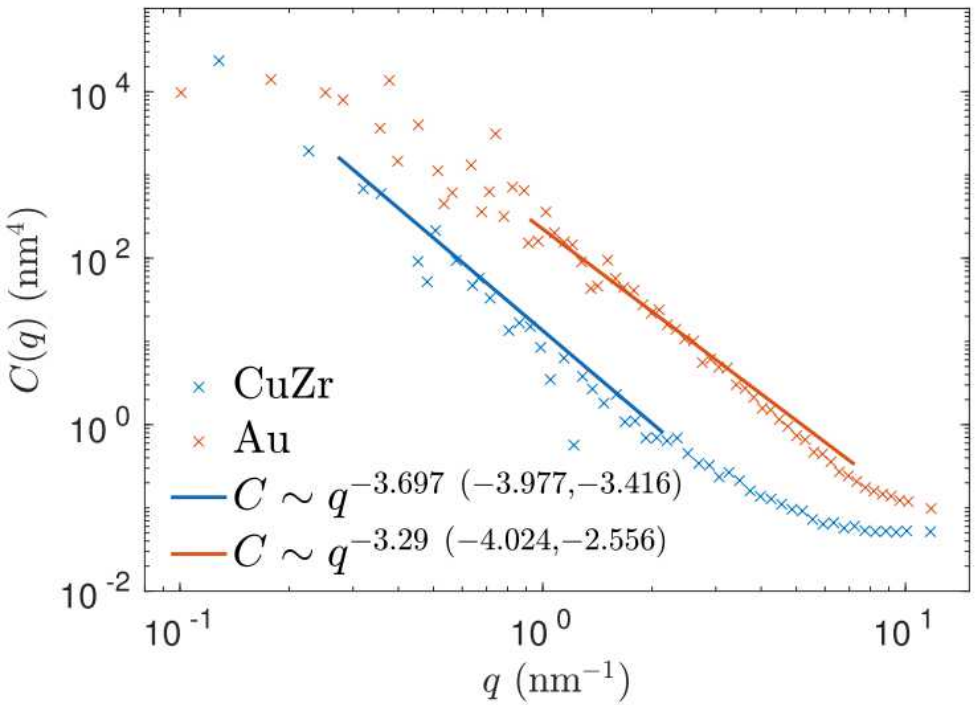


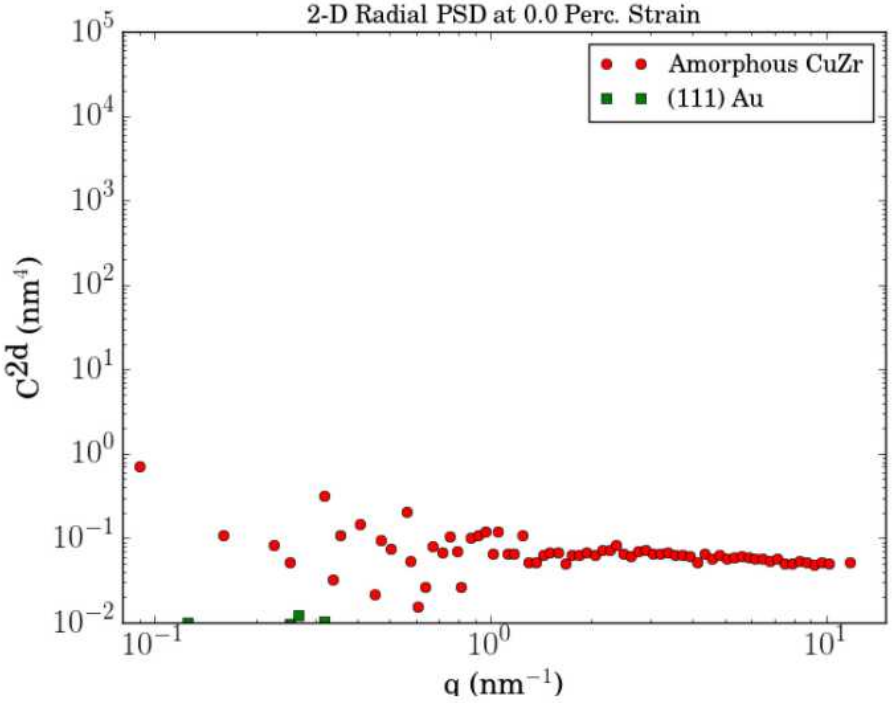



Amorphous CuZr
Au(111)
y
z
x
q_y (nm^{-1})
q_x (nm^{-1})
-10
-5
0
5
10
4
2
0
-2
-4

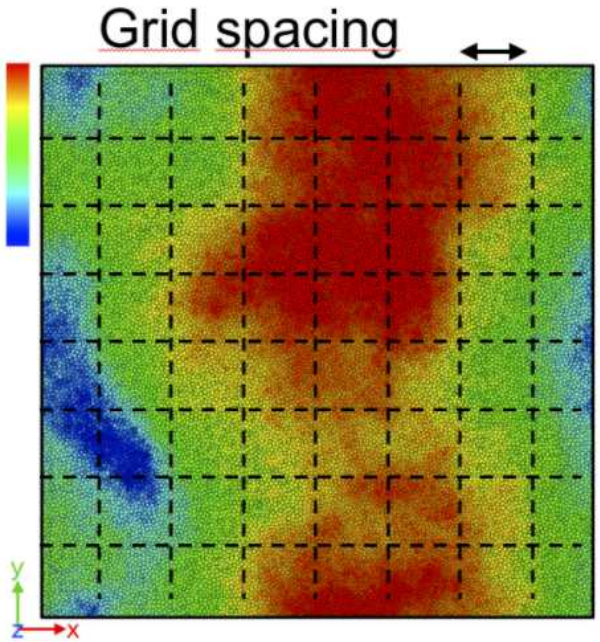
The radially averaged PSD for amorphous CuZr and Au(111)

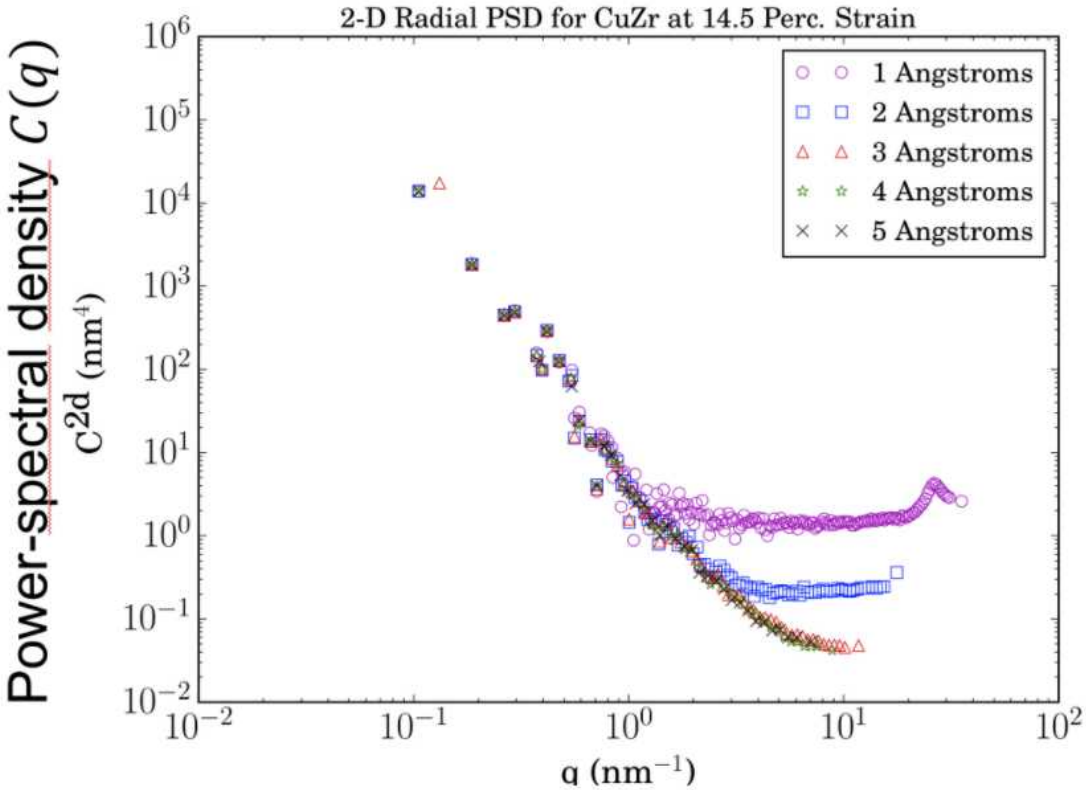
$$C(q) \sim q^{-2(1+H)}$$



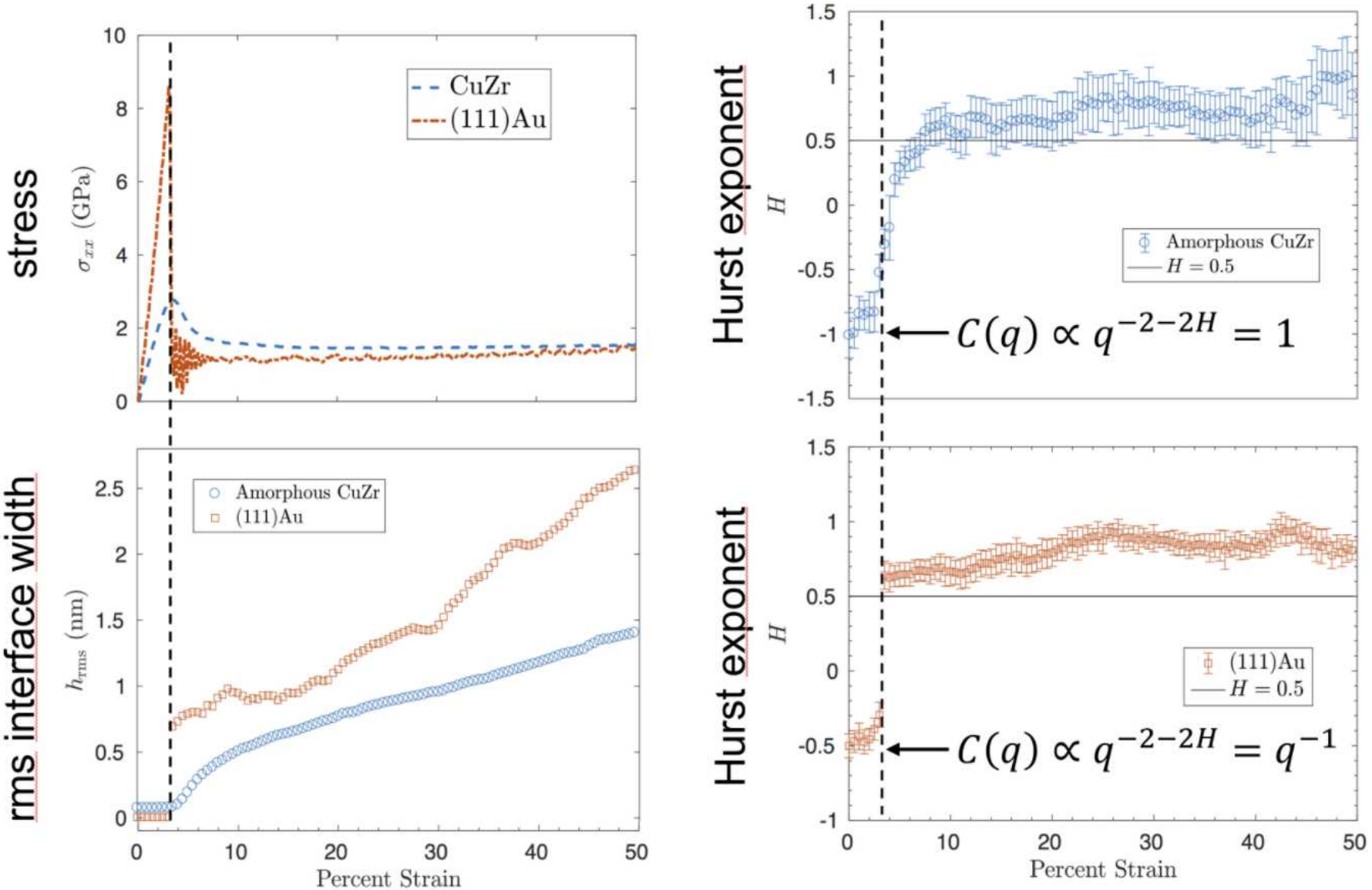


System size convergence and surface-grid convergence

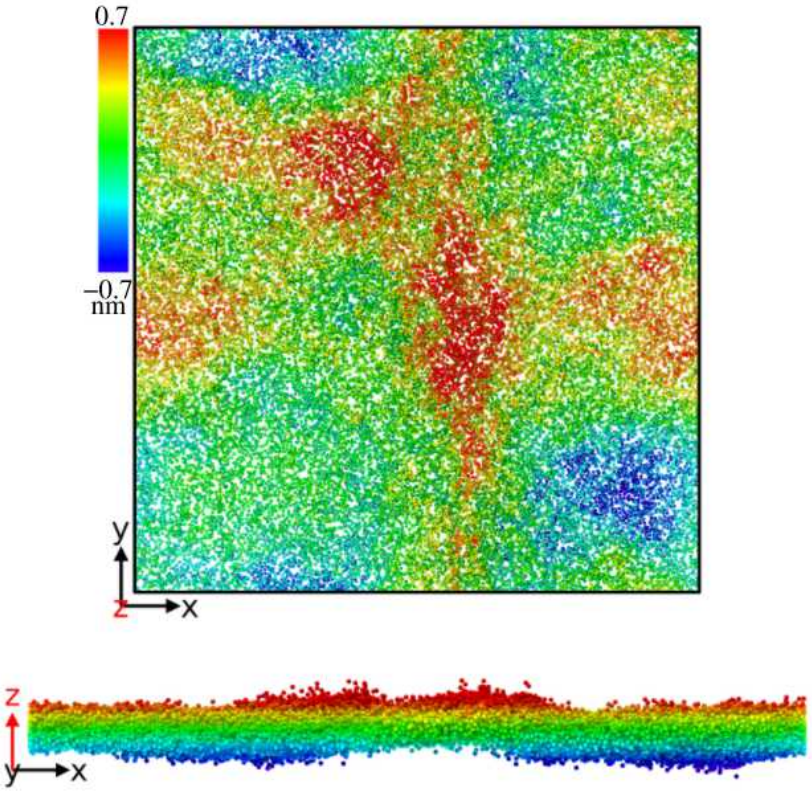


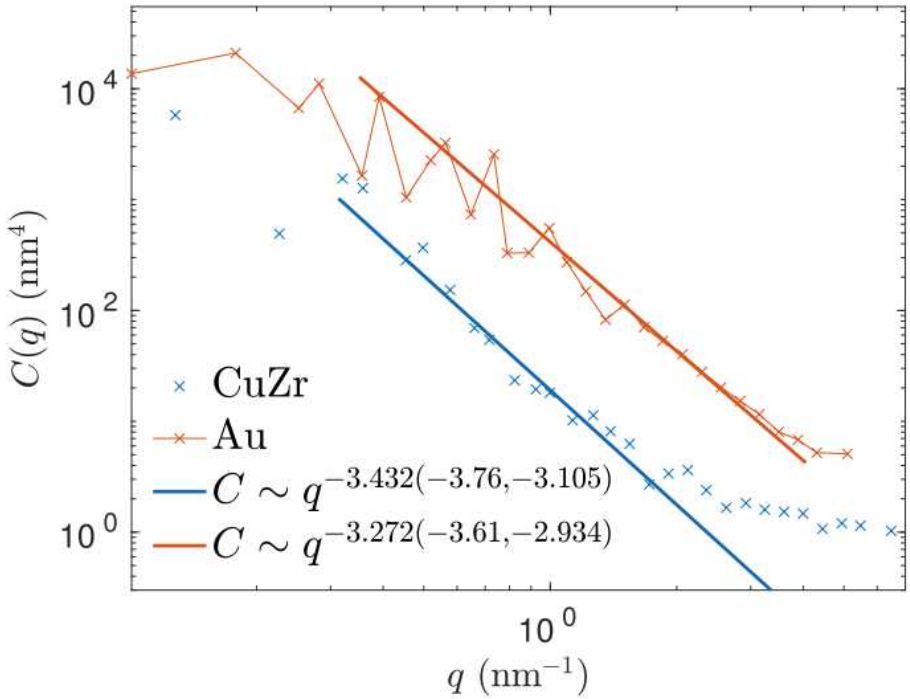


$C(q) \sim q^{-2(1+H)}$: H as a function of strain



PSD of plane of atoms within the bulk





Bulk zz-displacement correlation function and power-law scaling

3D displacements correlations

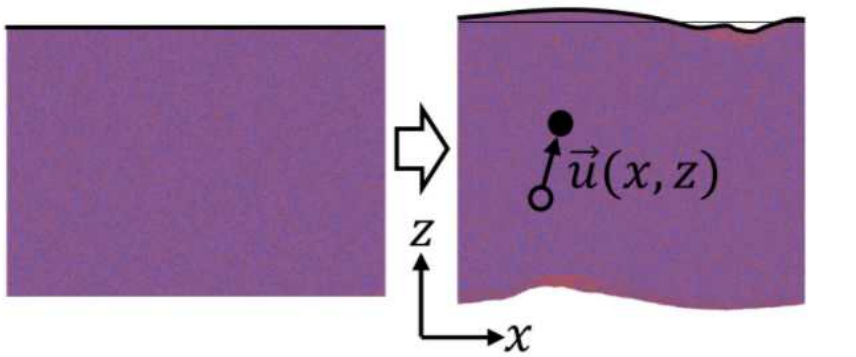
$$G_{zz}(\vec{r}) = \langle u_z(0) u_z(\vec{r}) \rangle$$

⇨ Fourier transform: $G_{zz}(\vec{q})$

2D in-plane correlations

$$C(q) \propto q G_{zz}(q)$$

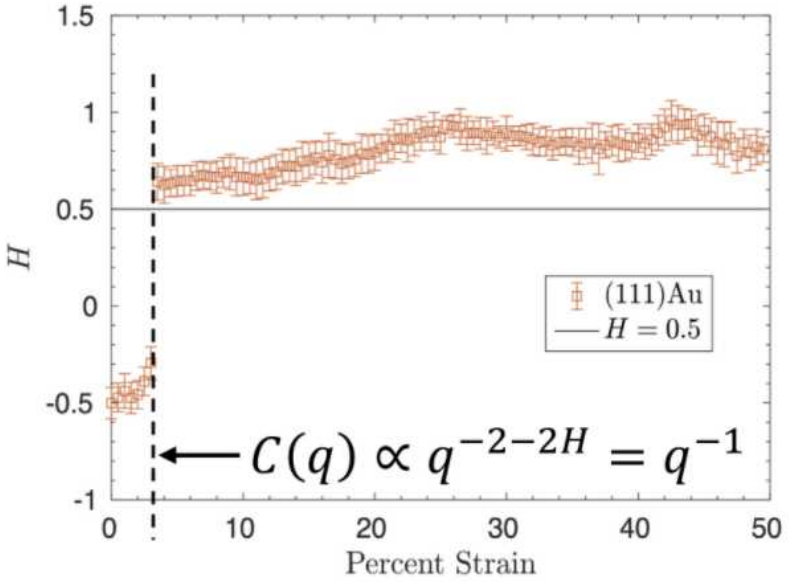
$$h(x) = u_z(x, z = 0)$$



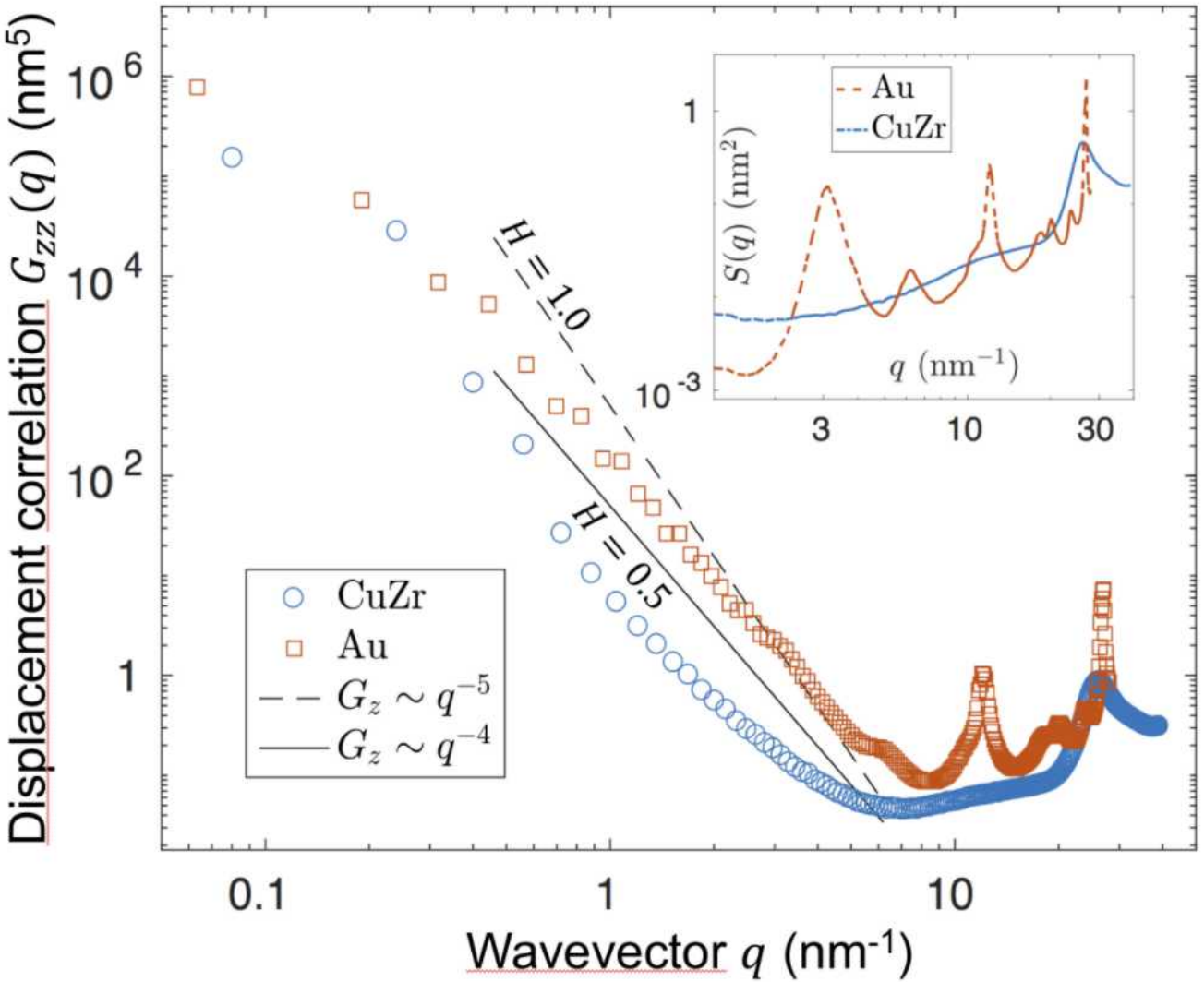
Elastic limit

$$G_{zz}(q) \propto q^{-2}$$

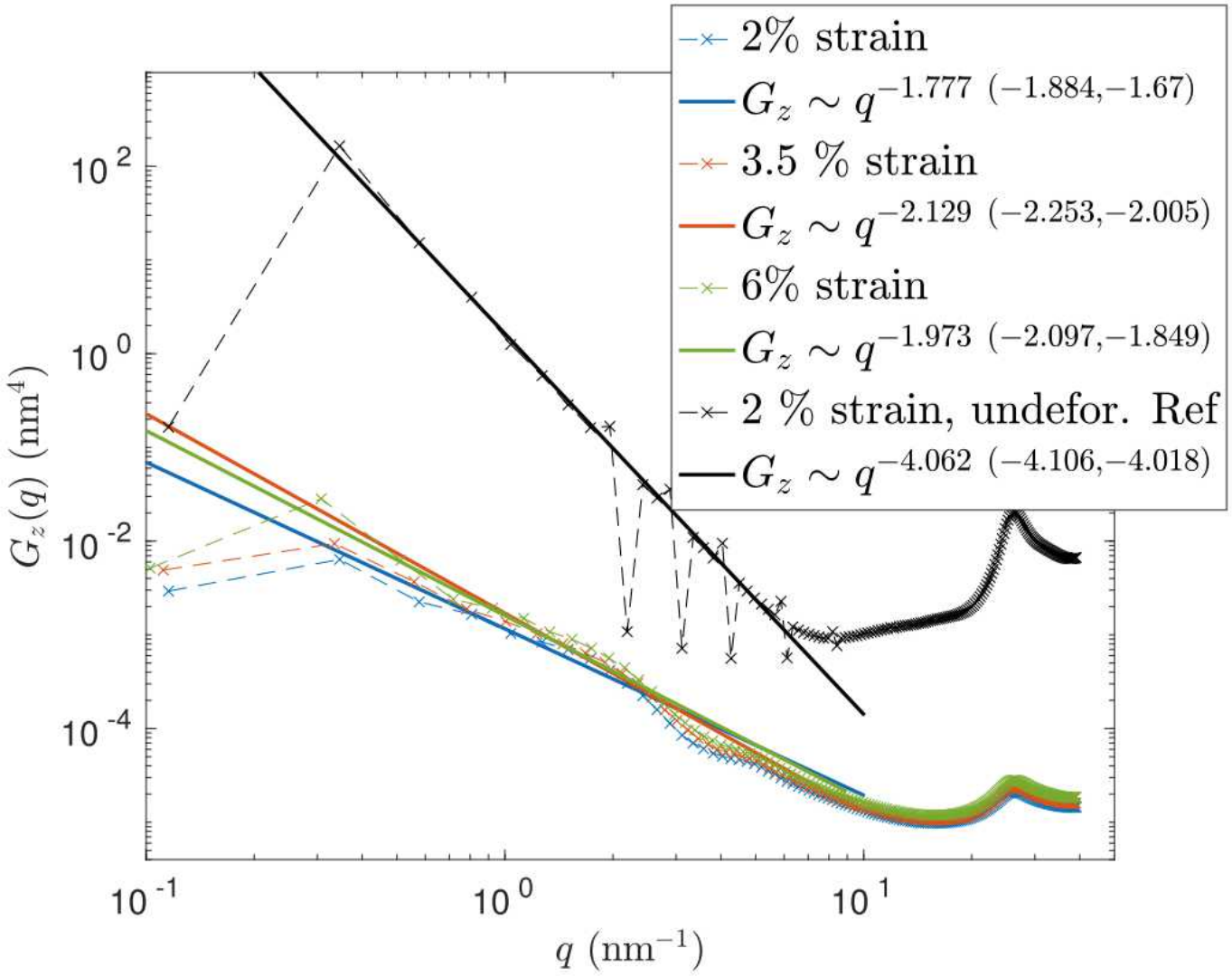
- structural disorder
  DiDonna, Lubensky, PRE 72, 066619 (2005)
- thermal disorder
  Campana, Müser, PRB 74, 075420 (2006)



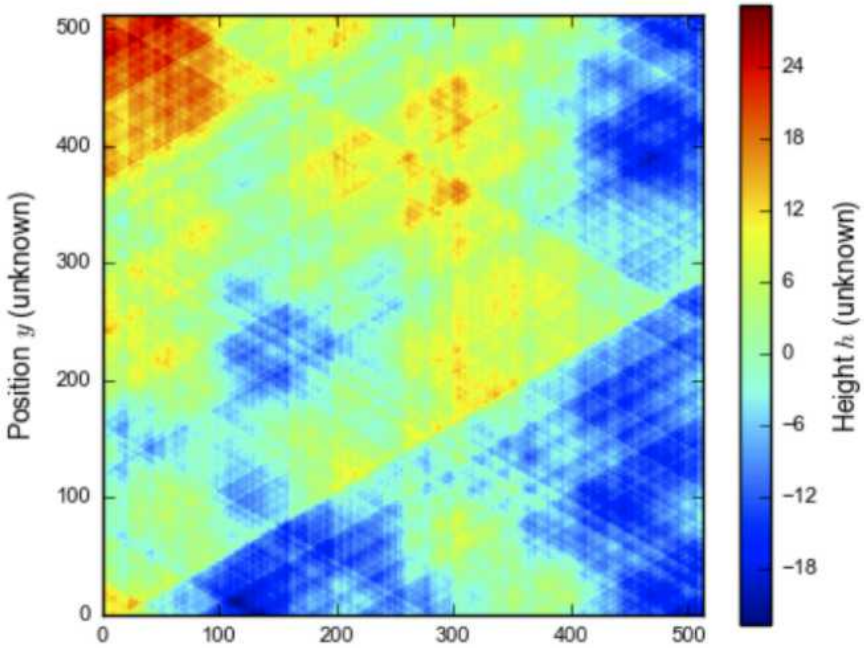
Bulk zz-displacement correlation function and power-law scaling

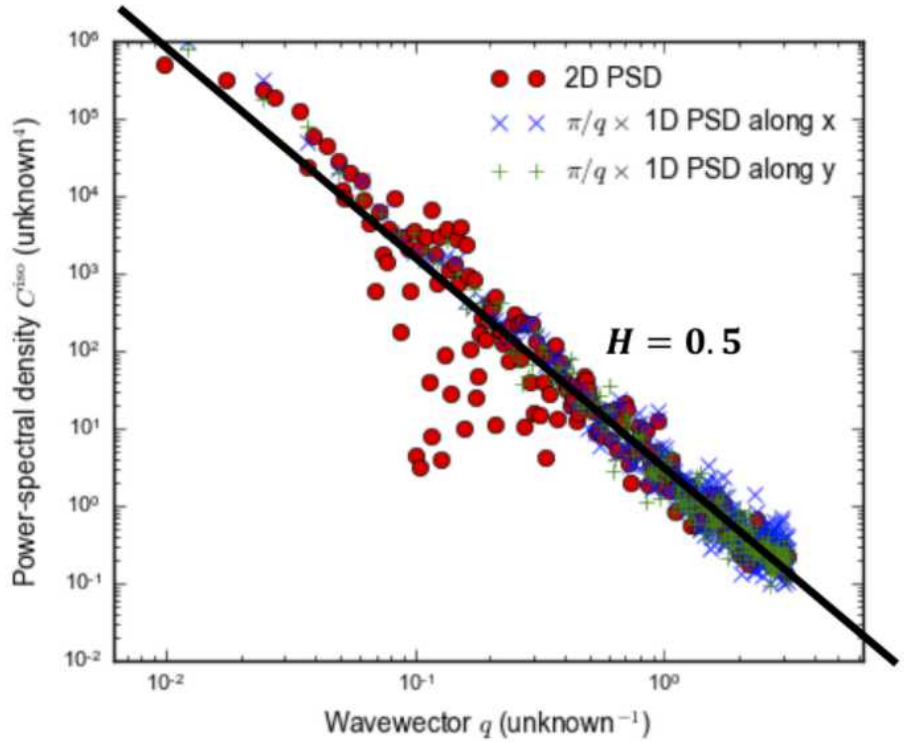


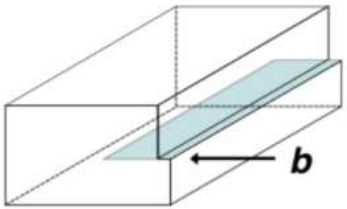
Bulk *elastic* zz-displacement correlation power-law scaling $G_z \sim q^{-2}$



Affect of surface steps







$FT\{\Theta(x)\} \propto 1/q \rightarrow$ 1D PSD $\propto 1/q^2 \rightarrow$ 2D PSD $\propto \frac{1}{q^3}$

self-affine 2D PSD $\propto 1/q^{2-2H}$

Future Work

- Understand the role of geometric factors (steps, kinks, etc.) on H and any bounds
- Implementation into continuum models with well defined yield criterion and constitutive law
- Wider array of amorphous solids and glasses. Currently looking at High Entropy Alloys —between crystal and amorphous

Acknowledgements

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