Contact mechanics and elements of tribology Lecture 4. Micromechanical contact: roughness

Vladislav A. Yastrebov

Mines Paris - PSL, CNRS Centre des Matériaux, Evry, France



@ Centre des Matériaux (& virtually) February 25, 2025



Creative Commons BY Vladislav A. Yastrebov

Outline

- Introduction
- Measurement techniques
- Classifications
- Main characteristics
- PDF and PSD
- Random process model of roughness
- Computational roughness models
- Reading

















- processing
- polishing
- coating
- microstructure
- surface energy
- deformation
- aging
- environment



- processing
- polishing
- coating
- microstructure
- surface energy
- deformation
- aging
- environment



Fig. Persistent slip marks [1]



Fig. Rumpling (thermal cycling induced roughness in air)[2]



Fig. Epitaxial surface growth [3,4] [1] J.Polák, J. Man & K. Orbtilk, Int J Fatigue 25 (2003) [2] V.K. Tolpygo, D.R. Clarke, Acta Mat 52 (2004) [3] M. Einax, W. Dieterich, P. Maass, Rev Mod Phys 85 (2013) [4] J.R. Arthur, Surf Sci 500 (2002)

- processing
- polishing
- coating
- microstructure
- surface energy
- deformation
- aging
- environment

Roughness affects:

- stress-strain state
- dry friction
- wear
- adhesion
- fluid flow
- sealing

energy transfer



Fig. True contact area and stress fluctuations

V.A. Yastrebov

- processing
- polishing
- coating
- microstructure
- surface energy
- deformation
- aging
- environment

Roughness affects:

- stress-strain state
- dry friction
- wear
- adhesion
- fluid flow
- sealing

energy transfer



Fig. True contact area and stress fluctuations

Roughness

Natural and industrial surfaces are *rough*:

- processing
- polishing
- coating
- microstructure
- surface energy
- deformation
- aging
- environment

Roughness affects:

- stress-strain state
- dry friction
- wear
- adhesion
- fluid flow
- sealing

V.A. Yastreboy



Fig. Numerical simulation of airflow around a (dimpled) golf ball [5]

Lecture 4

[5] C.E. Smith, PhD thesis (2011)

15/131

- processing
- polishing
- coating
- microstructure
- surface energy
- deformation
- aging
- environment

Roughness affects:

- stress-strain state
- dry friction
- wear
- adhesion
- fluid flow
- sealing

energy transfer





Fig. Fluid passage through free volume between rough surfaces







Temperature In plane heat flux Vertical heat flux Fig. Heat transfer between rough surfaces (asperity-based model)











Confusing representation that should be avoided:



Still Hertzian solution remains valid at asperity tips



Still Hertzian solution remains valid at asperity tips

- Stylus measurements
 - Mechanical contact of a tip with surface
 - Force $\geq 3\mu g$, tip radius $\geq 50 \text{ nm}$
 - Mainly for profile measurements *y*(*x*)

Optical measurements

- Confocal (laser scanning) microscopy - highest lateral resolution
- Interferometry (WLI):
 - highest vertical resolution
 - 10 to 100 times faster than CM
- Scanning Electronic Microscopy (SEM):
 - in secondary electron emission
 - electrons penetrate in the matter \rightarrow roughness smoothing
 - conducting materials
- Nano-contact measurements
 - Atomic Force Microscopy (AFM) roughness + adhesive and elastic properties
 - Scanning Tunneling Microscope (STM)

V.A. Yastrebov

Lecture 4





Valley measurement error

- Stylus measurements
 - Mechanical contact of a tip with surface
 - Force $\ge 3\mu g$, tip radius $\ge 50 \text{ nm}$
 - Mainly for profile measurements *y*(*x*)
- Optical measurements
 - Confocal (laser scanning) microscopy - highest lateral resolution
 - Interferometry (WLI):
 - highest vertical resolution
 - 10 to 100 times faster than CM
 - Scanning Electronic Microscopy (SEM):
 - in secondary electron emission
 - electrons penetrate in the matter \rightarrow roughness smoothing
 - conducting materials
- Nano-contact measurements
 - Atomic Force Microscopy (AFM) roughness + adhesive and elastic properties
 - Scanning Tunneling Microscope (STM)

V.A. Yastrebov

Stylus profilometer



Modern stylus profilometer www.bruker.com



Roughness measurements ($\Delta z \approx 30 \ \mu m$) www.icryst.com

- Stylus measurements
 - Mechanical contact of a tip with surface
 - Force $\ge 3\mu g$, tip radius $\ge 50 \text{ nm}$
 - Mainly for profile measurements *y*(*x*)
- Optical measurements
 - Confocal (laser scanning) microscopy - highest lateral resolution
 - Interferometry (WLI):
 - highest vertical resolution
 - 10 to 100 times faster than CM
 - Scanning Electronic Microscopy (SEM):
 - in secondary electron emission
 - electrons penetrate in the matter \rightarrow roughness smoothing
 - conducting materials
- Nano-contact measurements
 - Atomic Force Microscopy (AFM) roughness + adhesive and elastic properties
 - Scanning Tunneling Microscope (STM)

V.A. Yastrebov

Confocal microscopy Light source



Principle of confocal microscopy adapted from www.wikipedia.org

Stylus measurements

- Mechanical contact of a tip with surface
- Force $\ge 3\mu g$, tip radius $\ge 50 \text{ nm}$
- Mainly for profile measurements *y*(*x*)

Optical measurements

- Confocal (laser scanning) microscopy - highest lateral resolution
- Interferometry (WLI):
 - highest vertical resolution
 - 10 to 100 times faster than CM
- Scanning Electronic Microscopy (SEM):
 - in secondary electron emission
 - electrons penetrate in the matter \rightarrow roughness smoothing
 - conducting materials

Nano-contact measurements

- Atomic Force Microscopy (AFM)
 roughness + adhesive and elastic properties Stainless steel machined with micro-electric
- Scanning Tunneling Microscope (STM)

V.A. Yastrebov

Lecture 4

Confocal microscopy



1 euro surface www.wikipedia.org



(STM) discharge www.laserfocusworld.org

- Stylus measurements
 - Mechanical contact of a tip with surface
 - Force $\ge 3\mu g$, tip radius $\ge 50 \text{ nm}$
 - Mainly for profile measurements *y*(*x*)
- Optical measurements
 - Confocal (laser scanning) microscopy - highest lateral resolution
 - Interferometry (WLI):
 - highest vertical resolution
 - 10 to 100 times faster than CM
 - Scanning Electronic Microscopy (SEM):
 - in secondary electron emission
 - electrons penetrate in the matter \rightarrow roughness smoothing
 - conducting materials
- Nano-contact measurements
 - Atomic Force Microscopy (AFM) roughness + adhesive and elastic properties
 - Scanning Tunneling Microscope (STM)

V.A. Yastrebov

Lecture 4

White Light Interferometry



Diamond-turned optics www.zygo.com



US quarter surface www.zygo.com

- Stylus measurements
 - Mechanical contact of a tip with surface
 - Force $\geq 3\mu g$, tip radius $\geq 50 \text{ nm}$
 - Mainly for profile measurements *y*(*x*)
- Optical measurements
 - Confocal (laser scanning) microscopy - highest lateral resolution
 - Interferometry (WLI):
 - highest vertical resolution
 - 10 to 100 times faster than CM
 - Scanning Electronic Microscopy (SEM):
 - in secondary electron emission
 - electrons penetrate in the matter \rightarrow roughness smoothing
 - conducting materials
- Nano-contact measurements
 - Atomic Force Microscopy (AFM) roughness + adhesive and elastic properties
 - Scanning Tunneling Microscope (STM)

V.A. Yastrebov







Modern AFM www.bruker.com



Roughness and elastic moduli (color) of polymer blend www.bruker.com

Stylus measurements

- Mechanical contact of a tip with surface
- Force $\geq 3\mu g$, tip radius $\geq 50 \text{ nm}$
- Mainly for profile measurements *y*(*x*)

Optical measurements

- Confocal (laser scanning) microscopy - highest lateral resolution
- Interferometry (WLI):
 - highest vertical resolution
 - 10 to 100 times faster than CM
- Scanning Electronic Microscopy (SEM):
 - in secondary electron emission
 - electrons penetrate in the matter \rightarrow roughness smoothing
 - conducting materials

Nano-contact measurements

- Atomic Force Microscopy (AFM) roughness + adhesive and elastic properties
- Scanning Tunneling Microscope (STM)

V.A. Yastrebov



STM



Fig. Center for NanoScience logo imprinted at atomic scale

www.cens.de



Atomic steps on platinum surface (500×500 nm) www.icryst.com "The Surface-Topography Challenge: A Multi-Laboratory Benchmark Study to Advance the Characterization of Topography" just submitted

Roughness: classification



Fig. Roughness classification according to Nayak^[1]

[1] Nayak, J. Lub. Tech. (ASME) 93:398 (1971)

Roughness: classification



Fig. Roughness classification according to Nayak^[1]

[1] Nayak, J. Lub. Tech. (ASME) 93:398 (1971)

Roughness and geometry/form

- Roughness vs geometry of surfaces
- Sometimes macroscopic geometry is substracted (filtered out): form→error of form→wavyness→roughness
- Non-trivial to remove macroscopic shape
- Most roughness measurement tools enable shape removal



Fig. Circular metalic seal with turned copper surface^[1]

[1] F.P. Rafòls, Licentiate Thesis, LTU 2016.

V.A. Yastrebov

Lecture 4

Roughness and geometry/form

- Roughness vs geometry of surfaces
- Sometimes macroscopic geometry is substracted (filtered out): form→error of form→wavyness→roughness
- Non-trivial to remove macroscopic shape
- Most roughness measurement tools enable shape removal



Fig. (left) impact crater, (right) shape is filtered out

Lecture 4

Roughness and geometry/form

- Roughness vs geometry of surfaces
- Sometimes macroscopic geometry is substracted (filtered out): form→error of form→wavyness→roughness
- Non-trivial to remove macroscopic shape
- Most roughness measurement tools enable shape removal



Fig. (left) spherical indenter, (right) $z = a(x^2 + y^2)$ shape is substracted

Lecture 4

Integral quantities

■ Average of absolute values [l.u.] (profile - *R*_a, surface - *S*_a)

$$S_a = \frac{1}{A} \int_A |z(x,y) - \bar{z}| \, dA, \quad S_a = \frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N |z_{ij} - \bar{z}|$$
Integral quantities

■ Average of absolute values [l.u.] (profile - *R*_a, surface - *S*_a)

$$S_a = \frac{1}{A} \int_A |z(x,y) - \bar{z}| \, dA, \quad S_a = \frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N |z_{ij} - \bar{z}|$$

Standard deviation of height [l.u.] (σ or R_q for profile, S_q for surface)

$$\sigma = \sqrt{\frac{1}{A} \int_{A} (z(x,y) - \bar{z})^2 \, dA}, \quad \sigma = \frac{1}{N} \sqrt{\sum_{i=1}^{N} \sum_{j=1}^{N} (z_{ij} - \bar{z})^2}$$

Integral quantities

■ Average of absolute values [l.u.] (profile - *R*_a, surface - *S*_a)

$$S_a = \frac{1}{A} \int_A |z(x, y) - \bar{z}| \, dA, \quad S_a = \frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N |z_{ij} - \bar{z}|$$

Standard deviation of height [l.u.] (σ or R_q for profile, S_q for surface)

$$\sigma = \sqrt{\frac{1}{A} \int_{A} (z(x,y) - \bar{z})^2 \, dA}, \quad \sigma = \frac{1}{N} \sqrt{\sum_{i=1}^{N} \sum_{j=1}^{N} (z_{ij} - \bar{z})^2}$$

 Maximal valley depth R_v,S_v, maximal peak height R_p,S_p [l.u.] very sensitive to sample area

Integral quantities

■ Average of absolute values [l.u.] (profile - *R*_a, surface - *S*_a)

$$S_a = \frac{1}{A} \int_A |z(x, y) - \bar{z}| \, dA, \quad S_a = \frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N |z_{ij} - \bar{z}|$$

Standard deviation of height [l.u.] (σ or R_q for profile, S_q for surface)

$$\sigma = \sqrt{\frac{1}{A} \int_{A} (z(x,y) - \bar{z})^2 dA}, \quad \sigma = \frac{1}{N} \sqrt{\sum_{i=1}^{N} \sum_{j=1}^{N} (z_{ij} - \bar{z})^2}$$

- Maximal valley depth R_v,S_v, maximal peak height R_p,S_p [l.u.] very sensitive to sample area
- Skewness [adim] (γ_1 or R_{sk} , S_{sk})

$$\gamma_1 = \frac{1}{A\sigma^3} \int_A (z(x,y) - \bar{z})^3 dA, \qquad \gamma_1 = \frac{1}{N^2\sigma^3} \sum_{i=1}^N \sum_{j=1}^N (z_{ij} - \bar{z})^3$$

Main characteristics

Integral quantities

■ Average of absolute values [l.u.] (profile - *R*_a, surface - *S*_a)

$$S_a = \frac{1}{A} \int_A |z(x, y) - \bar{z}| \, dA, \quad S_a = \frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N |z_{ij} - \bar{z}|$$

Standard deviation of height [l.u.] (σ or R_q for profile, S_q for surface)

$$\sigma = \sqrt{\frac{1}{A} \int_{A} (z(x,y) - \bar{z})^2 \, dA}, \quad \sigma = \frac{1}{N} \sqrt{\sum_{i=1}^{N} \sum_{j=1}^{N} (z_{ij} - \bar{z})^2}$$

- Maximal valley depth R_v,S_v, maximal peak height R_p,S_p [l.u.] very sensitive to sample area
- Skewness [adim] (γ_1 or R_{sk} , S_{sk})

$$\gamma_1 = \frac{1}{A\sigma^3} \int_A (z(x,y) - \bar{z})^3 dA, \qquad \gamma_1 = \frac{1}{N^2 \sigma^3} \sum_{i=1}^N \sum_{j=1}^N (z_{ij} - \bar{z})^3$$

• Kurtosis [adim] (κ or R_{ku} , S_{ku})

$$\kappa = \frac{1}{A\sigma^4} \int\limits_A (z(x,y) - \bar{z})^4 \, dA,$$

$$\kappa = \frac{1}{N^2 \sigma^4} \sum_{i=1}^{N} \sum_{j=1}^{N} (z_{ij} - \bar{z})^4$$

V.A. Yastrebov

Lecture 4

40/131

Integral quantities II

Average of absolute value of gradient (slope) [adim] (profile - R_{da}, surface - S_{da})

$$S_{da} = \langle \left| \nabla z(x, y) - \overline{\nabla z} \right| \rangle = \frac{1}{A} \int_{A} \left| \nabla z(x, y) - \overline{\nabla z} \right| dA$$
$$S_{da} = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \left| \frac{z_{i+1,j} - z_{i,j} - \overline{\Delta z_x}}{\Delta x} \right| + \left| \frac{z_{i,j+1} - z_{i,j} - \overline{\Delta z_y}}{\Delta y} \right|$$

Integral quantities II

 Average of absolute value of gradient (slope) [adim] (profile - R_{da}, surface - S_{da})

$$S_{da} = \langle \left| \nabla z(x, y) - \overline{\nabla z} \right| \rangle = \frac{1}{A} \int_{A} \left| \nabla z(x, y) - \overline{\nabla z} \right| dA$$
$$S_{da} = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \left| \frac{z_{i+1,j} - z_{i,j} - \overline{\Delta z_x}}{\Delta x} \right| + \left| \frac{z_{i,j+1} - z_{i,j} - \overline{\Delta z_y}}{\Delta y} \right|$$

Standard deviation of gradient (slope) [adim] (profile - *R*_{dq}, surface - *S*_{dq})

$$S_{dq} = \sqrt{\langle \left| \nabla z(x,y) - \overline{\nabla z} \right|^2 \rangle} = \sqrt{\frac{1}{A} \int_A \left| \nabla z(x,y) - \overline{\nabla z} \right|^2 dA}$$
$$S_{dq} = \sqrt{\frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N \left| \frac{z_{i+1,j} - z_{i,j} - \overline{\Delta z_x}}{\Delta x} \right| + \left| \frac{z_{i,j+1} - z_{i,j} - \overline{\Delta z_y}}{\Delta y} \right|^2}$$

Main characteristics II

Integral quantities II

 Average of absolute value of gradient (slope) [adim] (profile - R_{da}, surface - S_{da})

$$S_{da} = \langle \left| \nabla z(x, y) - \overline{\nabla z} \right| \rangle = \frac{1}{A} \int_{A} \left| \nabla z(x, y) - \overline{\nabla z} \right| dA$$
$$S_{da} = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \left| \frac{z_{i+1,j} - z_{i,j} - \overline{\Delta z}_x}{\Delta x} \right| + \left| \frac{z_{i,j+1} - z_{i,j} - \overline{\Delta z}_y}{\Delta y} \right|$$

Standard deviation of gradient (slope) [adim] (profile - R_{dq}, surface - S_{dq})

$$S_{dq} = \sqrt{\left\langle \left| \nabla z(x,y) - \overline{\nabla z} \right|^2 \right\rangle} = \sqrt{\frac{1}{A}} \int_A \left| \nabla z(x,y) - \overline{\nabla z} \right|^2 dA$$
$$S_{dq} = \sqrt{\frac{1}{N^2}} \sum_{i=1}^N \sum_{j=1}^N \left| \frac{z_{i+1,j} - z_{i,j} - \overline{\Delta z_x}}{\Delta x} \right| + \left| \frac{z_{i,j+1} - z_{i,j} - \overline{\Delta z_y}}{\Delta y} \right|^2$$

• Often in integrated slope measurements a smoothing filter is used, for example, according to ASME B46.1 standard

$$\frac{\partial z}{\partial x} \approx \frac{1}{60\Delta x} (z_{i+3,j} - 9z_{i+2,j} + 45z_{i+1,j} - 45z_{i-1,j} + 9z_{i-2,j} - z_{i-3,j})$$

V.A. Yastrebov

Lecture 4

43/131

Main characteristics: probability density

- Probability density of heights P(z)
- Properties and moments

$$1 = \int_{-\infty}^{\infty} P(z) dz, \qquad \bar{z} = \int_{-\infty}^{\infty} zP(z) dz, \qquad \sigma = \sqrt{\int_{-\infty}^{\infty} (z - \bar{z})^2 P(z) dz}$$
$$\mu_q = \int_{-\infty}^{\infty} z^q P(z) dz \quad \text{then} \quad \mu_0 = 1, \ \mu_1 = \bar{z}, \ \mu_2 = \sigma^2 + \bar{z}^2$$

Link to skewness



Main characteristics: probability density II

Distribution examples

Normal (Gaussian):
$$P(x, \mu, \sigma) = \frac{1}{\sigma \sqrt{2\pi}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right], x \in \mathbb{R}$$



Main characteristics: probability density II

Distribution examples



Main characteristics: probability density II

Distribution examples

• Weibull:
$$P(x, k, \lambda) = \frac{k}{\lambda} \left(\frac{x}{\lambda}\right)^{k-1} \exp{-(x/\lambda)^k} x \in \mathbb{R}^+$$



- Turning, scratching, shaping changes macroscopic distribution P_{macro} but might keep microscopic distribution intact P_{micro}
- Wear, polishing, flattening results in removal of the right distribution tail $P(z > z_0) \rightarrow 0$: negative skewness



Macro- and microscopic roughness (left: diamond-turned surface, right: cross-hatched surface) Images from www.zygo.com used

Main characteristics: comments on PDF

- Turning, scratching, shaping changes macroscopic distribution P_{macro} but might keep microscopic distribution intact P_{micro}
- Wear, polishing, flattening results in removal of the right distribution tail $P(z > z_0) \rightarrow 0$: negative skewness



Pérez-Ràfols, Larsson, Almqvist, Tribol Int 94 (2016)

- Turning, scratching, shaping changes macroscopic distribution P_{macro} but might keep microscopic distribution intact P_{micro}
- Wear, polishing, flattening results in removal of the right distribution tail $P(z > z_0) \rightarrow 0$: negative skewness



Initial surface with Gaussian PDF and surface after polishing

- Turning, scratching, shaping changes macroscopic distribution P_{macro} but might keep microscopic distribution intact P_{micro}
- Wear, polishing, flattening results in removal of the right distribution tail $P(z > z_0) \rightarrow 0$: negative skewness



Very fresh asphalt concrete

Normal asphalt concrete

- Turning, scratching, shaping changes macroscopic distribution P_{macro} but might keep microscopic distribution intact P_{micro}
- Wear, polishing, flattening results in removal of the right distribution tail $P(z > z_0) \rightarrow 0$: negative skewness



Very fresh asphalt concrete

Normal asphalt concrete . . . with a bolt ©

- Turning, scratching, shaping changes macroscopic distribution P_{macro} but might keep microscopic distribution intact P_{micro}
- Wear, polishing, flattening results in removal of the right distribution tail $P(z > z_0) \rightarrow 0$: negative skewness



Old asphalt concrete with worn out bitumen

- Turning, scratching, shaping changes macroscopic distribution P_{macro} but might keep microscopic distribution intact P_{micro}
- Wear, polishing, flattening results in removal of the right distribution tail $P(z > z_0) \rightarrow 0$: negative skewness



Atlas of machined surfaces (with height distributions)

Continuous autocorrelation function

$$R(\Delta x, \Delta y) = \lim_{L \to \infty} \frac{1}{L^2} \int_0^L \int_0^L z(x + \Delta x, y + \Delta y) z(x, y) \, dx dy$$

$$R(\Delta x, \Delta y) = \frac{1}{N^2} \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} z(x + \Delta x, y + \Delta y) z(x, y)$$



Continuous autocorrelation function

$$R(\Delta x, \Delta y) = \lim_{L \to \infty} \frac{1}{L^2} \int_0^L \int_0^L z(x + \Delta x, y + \Delta y) z(x, y) \, dx dy$$

$$R(\Delta x, \Delta y) = \frac{1}{N^2} \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} z(x + \Delta x, y + \Delta y) z(x, y)$$



Continuous autocorrelation function

$$R(\Delta x, \Delta y) = \lim_{L \to \infty} \frac{1}{L^2} \int_0^L \int_0^L z(x + \Delta x, y + \Delta y) z(x, y) \, dx dy$$

$$R(\Delta x, \Delta y) = \frac{1}{N^2} \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} z(x + \Delta x, y + \Delta y) z(x, y)$$



Continuous autocorrelation function

$$R(\Delta x, \Delta y) = \lim_{L \to \infty} \frac{1}{L^2} \int_0^L \int_0^L z(x + \Delta x, y + \Delta y) z(x, y) \, dx dy$$

$$R(\Delta x, \Delta y) = \frac{1}{N^2} \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} z(x + \Delta x, y + \Delta y) z(x, y)$$



Power spectral density (PSD)

Recall: Fourier Transform:
$$\hat{f}(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) \exp(-ikx) dx$$

- Recall: Discrete Fourier Transform: $\hat{f}_k = \sum_{n=0}^{N-1} x_n \exp(-ikn/N)$
- where *x* is the spatial coordinate, $k = 2\pi/\lambda$ is the wavenumber and λ is the wavelength.
- PSD is the Fourier Transform of *R* $\Phi(k_x, k_y) \equiv \hat{R}(k_x, k_y) = \text{FFT}[z(x + \Delta x, y + \Delta y) * z(x, y)]$
- Using convolution theorem

 $\Phi(k_x, k_y) = \hat{z}(k_x, k_y) \ \hat{z}^*(k_x, k_y) = \hat{z}^2(k_x, k_y)$

- Interpretation: energy distribution by frequencies
- Usage: signal analysis, seismology, microstructure characterization, roughness.

Spectral moments

Spectral moment m_{pq} , $p, q \in \mathbb{N}$:

$$m_{pq} = \iint_{-\infty}^{\infty} k_x^p k_y^q \Phi(k_x, k_y) \, dk_x dk_y$$

- Generalized spectral moment m_{pq} , $p, q \in \mathbb{R}^+$
- For isotropic surface: $m_2 = m_{20} = m_{02}$, $m_4 = 3m_{22} = m_{40} = m_{04}$
- Averaging:

$$m_2 = \frac{m_{20} + m_{02}}{2}, \quad m_4 = \frac{m_{40} + 3m_{22} + m_{04}}{3}$$

Physical meaning:

Height variance¹: $m_0 = \langle (z - \langle z \rangle)^2 \rangle$ Gradient variance: $2m_2 = \langle (\nabla z - \langle \nabla z \rangle)^2 \rangle$ Curvature variance: $m_4 = \langle (\nabla \cdot \nabla z - \langle \nabla \cdot \nabla z \rangle)^2 \rangle$

 Longuet-Higgins, M. S. (1957). The statistical analysis of a random, moving surface. Phil. Trans. Royal Society of London. Series A 249(966):321-387.
Nayak, P. R. (1971). Random Process Model of Rough Surfaces. Journal of Lubrication Technology, 93(3):398-407

¹Variance is a squared standard deviation

Lecture 4

- Fractal (self-affine) roughness
- Power spectral density (PSD) $\Phi(k) \sim k^{-2(H+1)}$

k is a wavenumber, H is the Hurst exponent.

- Isotropic/anisotropic surfaces
- **Gaussian**/non-Gaussian height distribution *P*(*h*)



- Fractal (self-affine) roughness
- Power spectral density (PSD) $\Phi(k) \sim k^{-2(H+1)}$

k is a wavenumber, *H* is the Hurst exponent.

- Isotropic/anisotropic surfaces
- **Gaussian**/non-Gaussian height distribution *P*(*h*)



- Fractal (self-affine) roughness
- Power spectral density (PSD) $\Phi(k) \sim k^{-2(H+1)}$

k is a wavenumber, H is the Hurst exponent.

- Isotropic/anisotropic surfaces
- **Gaussian**/non-Gaussian height distribution *P*(*h*)



Fig. Power spectral density, measurements

[1] Majumdar, Tien, Wear 136 (1990)

[2] Schmittbuhl, Jørgen Måløy, Phys. Rev. Lett. 78 (1997)

[3] Vallet, Lasseux, Sainsot, Zahouani, Tribol. Int. 42 (2009)

- Fractal (self-affine) roughness
- Power spectral density (PSD) $\Phi(k) \sim k^{-2(H+1)}$

k is a wavenumber, H is the Hurst exponent.

- Isotropic/anisotropic surfaces
- **Gaussian**/non-Gaussian height distribution *P*(*h*)



Adapted from

[4] Renard, Candela, Bouchaud, Geophys. Res. Lett. 40 (2013)

- Fractal (self-affine) roughness
- Power spectral density (PSD) $\Phi(k) \sim k^{-2(H+1)}$

k is a wavenumber, H is the Hurst exponent.

- Isotropic/anisotropic surfaces
- **Gaussian**/non-Gaussian height distribution *P*(*h*)



- Fractal (self-affine) roughness
- Power spectral density (PSD) $\Phi(k) \sim k^{-2(H+1)}$

k is a wavenumber, H is the Hurst exponent.

- Isotropic/anisotropic surfaces
- **Gaussian**/non-Gaussian height distribution *P*(*h*)
- Characteristics:
 - $\sqrt{\langle z^2 \rangle}$ rms heights
 - $\sqrt{\langle |\nabla z|^2 \rangle}$ rms slope (surface gradient)
 - $\alpha = m_{00}m_{40}/m_{20}^2$ breadth of the spectrum (Nayak's parameter^[B]),

spectral moments $m_{pq} = \int_{-\infty}^{\infty} k_x^p k_y^q \Phi(k_x, k_y) dk_x dk_y$

Random process theory

[A] Longuet-Higgins, Philos. Trans. R. Soc. A 250:157 (1957) [B] Nayak, J. Lub. Tech. (ASME) 93:398 (1973) [C] Greenwood, Wear 261: 191 (2006) [D] Borri, Paggi, J. Phys. D Appl Phys 48:045301 (2015) V.A. Yastrebov Lecture 4



- Fractal (self-affine) roughness
- Power spectral density (PSD) $\Phi(k) \sim k^{-2(H+1)}$

k is a wavenumber, *H* is the Hurst exponent.

- Isotropic/anisotropic surfaces
- **Gaussian**/non-Gaussian height distribution *P*(*h*)
- Characteristics:
 - $\sqrt{\langle z^2 \rangle}$ rms heights
 - $\sqrt{\langle |\nabla z|^2 \rangle}$ rms slope (surface gradient)
 - $\alpha = m_{00}m_{40}/m_{20}^2$ breadth of the spectrum (Nayak's parameter^[B]),

spectral moments $m_{pq} = \int_{-\infty}^{\infty} k_x^p k_y^q \Phi(k_x, k_y) dk_x dk_y$

Random process theory

[A] Longuet-Higgins, Philos. Trans. R. Soc. A 250:157 (1957) [B] Nayak, J. Lub. Tech. (ASME) 93:398 (1973) [C] Greenwood, Wear 261: 191 (2006) [D] Borri, Paggi, J. Phys. D Appl Phys 48:045301 (2015) V.A. Yastrebov Lecture 4







Flight over a rough surface



Romanesco broccoli

Mandelbrot set (not a fractal)

Recursive function

$$z_{i+1}=z_i^2+z,\quad z\in\mathbb{C}$$



Mandelbrot set (not a fractal)

Recursive function

$$z_{i+1} = z_i^2 + z, \quad z \in \mathbb{C}$$


Mandelbrot set (not a fractal)

$$z_{i+1} = z_i^2 + z, \quad z \in \mathbb{C}$$



Mandelbrot set (not a fractal)

$$z_{i+1} = z_i^2 + z, \quad z \in \mathbb{C}$$



Mandelbrot set (not a fractal)

$$z_{i+1} = z_i^2 + z, \quad z \in \mathbb{C}$$



Mandelbrot set (not a fractal)

$$z_{i+1} = z_i^2 + z, \quad z \in \mathbb{C}$$



Mandelbrot set (not a fractal)

$$z_{i+1} = z_i^2 + z, \quad z \in \mathbb{C}$$





Mandelbrot set (Wikipedia)



Element of Mandelbrot set (Wikipedia)



Element of Mandelbrot set (Wikipedia)



Element of Mandelbrot set (Wikipedia)



Element of Mandelbrot set (Wikipedia)



Element of Mandelbrot set (Wikipedia)

See animation



https://youtu.be/pCpLWbHVNhk 70 minutes of 4K "Eye of the Universe - Mandelbrot Fractal Zoom" e^{1091}

V.A. Yastrebov

Lecture 4

Real space

Fourier space



White noise, r_{ii}

[1] Y. Z. Hu and K. Tonder, Int. J. Machine Tools Manuf. 32, 83 (1992)

V.A. Yastrebov

Lecture 4

85/131



[1] Y. Z. Hu and K. Tonder, Int. J. Machine Tools Manuf. 32, 83 (1992)

V.A. Yastrebov

Lecture 4



[1] Y. Z. Hu and K. Tonder, Int. J. Machine Tools Manuf. 32, 83 (1992)

V.A. Yastrebov

Lecture 4

87/131





Synthesized rough surfaces: in equations

White noise:

 $w(x_i,y_j), \quad \langle w\rangle = 0, \quad \langle w^2\rangle = \Phi_0$

Transform in Fourier space:

$$\hat{w}_{ij} = \hat{w}(k_x, k_y) = \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} w(x_i, y_i) \exp[-i(k_x x_i + k_y y_j)], \quad \langle \hat{w}\hat{w}^* \rangle = \langle w^2 \rangle = \Phi_0$$

Create a filter

$$\hat{f}_{ij} = \hat{f}(k_x, k_y) = \begin{cases} \left[\frac{K_x^2 + K_y^2}{k_l^2}\right]^{-(1+H)/2}, \text{ for } 1 \le \frac{\sqrt{K_x^2 + K_y^2}}{k_l} \le \zeta \\ 0, \text{ elsewhere,} \end{cases},$$

where $K_x = (s+1)\pi/L - sk_x$, $K_y = (t+1)\pi/L - tk_y$ for $s, t \in \{-1, 1\}$, $\zeta = k_s/k_l$

Filter white noise:

$$\hat{z}_{ij} = \hat{z}(k_x, k_y) = \Re(\hat{f}_{ij}) \left[\Re(\hat{w}_{ij}) + \mathrm{i}\,\Im(\hat{w}_{ij}) \right]$$

Back to real space:

$$z(x_i, y_j) = \sum_{l=0}^{N-1} \sum_{m=0}^{N-1} \hat{z}_{lm} \exp[i2\pi(lx_i + my_j)/L]$$

Synthesized rough surfaces: in equations II

Power spectral density:

 $\Phi(k_x,k_y) = \hat{z}(k_x,k_y)\hat{z}^*(k_x,k_y) = \hat{f}^2(k_x,k_y)\hat{w}^2(k_x,k_y)$

Averaging over multiple samples:

$$\langle \Phi(k_x, k_y) \rangle = \langle \hat{w}^2(k_x, k_y) \rangle \hat{f}^2(k_x, k_y) = \begin{cases} \Phi_0 \left[\frac{\sqrt{K_x^2 + K_y^2}}{k_l} \right]^{-2(1+H)}, \text{ for } 1 \le \frac{\sqrt{K_x^2 + K_y^2}}{k_l} \le \zeta \\ 0, \text{ elsewhere,} \end{cases}$$

For isotropic surface:

$$\langle \Phi(K) \rangle = \begin{cases} \Phi_0(K/k_l)^{-2(1+H)}, & \text{if } 1 \le K/k_l \le \zeta \\ 0, & \text{otherwise.} \end{cases}$$

• Effect of the high frequency cutoff *k*_s



• Effect of the high frequency cutoff *k*_s



• Effect of the high frequency cutoff *k*_s



• Effect of the high frequency cutoff k_s



• Effect of the high frequency cutoff k_s



• Effect of the lower frequency cutoff k_l for $k_s/k_l = \text{const}$



Fig. Power spectral density (Fourier space) and corresponding rough surface (real space) for $k_l = 1$, $k_s = 43$

• Effect of the lower frequency cutoff k_l for $k_s/k_l = \text{const}$



Fig. Power spectral density (Fourier space) and corresponding rough surface (real space) for $k_I = 4$, $k_s = 171$

• Effect of the lower frequency cutoff k_l for $k_s/k_l = \text{const}$



Fig. Power spectral density (Fourier space) and corresponding rough surface (real space) for $k_l = 12$, $k_s = 512$

• Effect of the ratio of the higher cutoff to the discretization k_s/N



• Effect of the ratio of the higher cutoff to the discretization k_s/N



V.A. Yastrebov

Lecture 4

101/131

• Effect of the discretisation (single asperity)



Displacement Fig. Effect of the mesh on mechanical response

• Data interpolation (Shanon, bi-cubic Bézier surfaces) Experimental Smoothed (enriched)



Fig. Bi-cubic Bézier interpolation of an experimental rough surface

[1]Hyun, Robbins, Tribol. Int. (2007) [2] Yastrebov, Durand, Proudhon, Cailletaud, C.R. Mécan. (2011)

V.A. Yastrebov

Lecture 4

Effect of parameters

Effect of parameters:

- k_l low frequency cutoff - representativity/normality^[1,2,3]
- k_s high frequency cutoff - smoothness and density of asperities
- $\zeta = k_s/k_l \operatorname{ratio}^{[3]}$
 - breadth of the spectrum

 $\alpha \sim \zeta^{2H}$

- Nayak's parameter α is the central characteristic of roughness in asperity based mechanical models.
- [1] Vallet, Lasseux, Sainsot, Zahouani, Tribol. Int. (2009)
- [2] Yastreboy, Durand, Proudhon, Cailletaud, C.R. Mécan, (2011)
- [3] Yastrebov, Anciaux, Molinari, Phys. Rev. E (2012)
- [4] Yastreboy, Anciaux, Molinari, Int. J. Solids Struct. (2015)



Effect of parameters

Effect of parameters:

- *k_l* low frequency cutoff
 representativity/normality^[1,2,3]
- *k_s* high frequency cutoff
 smoothness and density of asperities
- $\Box \zeta = k_s / k_l \text{ ratio}^{[3]}$
 - breadth of the spectrum

 $\alpha \sim \zeta^{2H}$

- Nayak's parameter α is the central characteristic of roughness in asperity based mechanical models.
- [1] Vallet, Lasseux, Sainsot, Zahouani, Tribol. Int. (2009)
- [2] Yastrebov, Durand, Proudhon, Cailletaud, C.R. Mécan. (2011)
- [3] Yastrebov, Anciaux, Molinari, Phys. Rev. E (2012)
- [4] Yastrebov, Anciaux, Molinari, Int. J. Solids Struct. (2015)



V.A. Yastrebov

Lecture 4

105/131

Effect of parameters

Effect of parameters:

- *k_l* low frequency cutoff
 representativity/normality^[1,2,3]
- *k_s* high frequency cutoff
 smoothness and density of asperities
- $\Box \zeta = k_s / k_l \text{ ratio}^{[3]}$
 - breadth of the spectrum

 $\alpha \sim \zeta^{2H}$

- Nayak's parameter α is the central characteristic of roughness in asperity based mechanical models.
- [1] Vallet, Lasseux, Sainsot, Zahouani, Tribol. Int. (2009)
- [2] Yastrebov, Durand, Proudhon, Cailletaud, C.R. Mécan. (2011)
- [3] Yastrebov, Anciaux, Molinari, Phys. Rev. E (2012)
- [4] Yastrebov, Anciaux, Molinari, Int. J. Solids Struct. (2015)



V.A. Yastrebov

106/131

Interconnection of parameters

■ Spectral moment and *k*_l, *k*_s, *H*:

$$m_{0p} \approx m_{p0} \approx \Phi_0 \int_{k_l}^{k_s} \int_{0}^{2\pi} \left[k \cos(\varphi) \right]^p (k/k_l)^{-2(1+H)} k dk d\varphi = \Phi_0 k_l^{p+2} \frac{\zeta^{p-2H} - 1}{p - 2H} T(p)$$

with
$$T(p) = \int_{0}^{2\pi} \cos^{p}(\varphi) d\varphi = \begin{cases} 2\pi, & \text{if } p = 0; \\ \pi, & \text{if } p = 2; \\ 3\pi/4, & \text{if } p = 4. \end{cases}$$

Nayak's parameter

$$\alpha(H,\zeta) = \frac{3}{2} \frac{(1-H)^2}{H(H-2)} \frac{(\zeta^{-2H}-1)(\zeta^{4-2H}-1)}{(\zeta^{2-2H}-1)^2}$$

Asperity density

$$D = \frac{\sqrt{3}}{18\pi} \frac{m_4}{m_2} = \frac{\sqrt{3}}{24\pi} \frac{1-H}{2-H} \frac{\zeta^{4-2H}-1}{\zeta^{2-2H}-1} k_l^2$$

Interconnection of parameters



Numerical verification on 100 000 generated rough surfaces with 2048×2048 points
Interconnection of parameters



Interconnection of parameters



Detect summits (*z_{ij}* higher than neighbouring points) and evaluate second derivatives

$$\frac{\partial^2 z}{\partial x^2} = \frac{z_{i+1j} + z_{i-1j} - 2z_{ij}}{2\Delta x^2}; \quad \frac{\partial^2 z}{\partial y^2} = \frac{z_{i+1j} + z_{i-1j} - 2z_{ij}}{2\Delta x^2}$$
$$\frac{\partial^2 z}{\partial x \partial y} = \frac{z_{i+1j+1} + z_{i+1j+1} - z_{i+1j-1} - z_{i-1j+1}}{4\Delta x^2}$$

Principal curvatures $\kappa_{1,2}$:

$$\kappa_{1,2} = \frac{1}{2} \left(\frac{\partial^2 z}{\partial x^2} + \frac{\partial^2 z}{\partial y^2} \right) \pm \sqrt{ \left(\frac{\partial^2 z}{\partial x \partial y} \right)^2 + \frac{1}{4} \left(\frac{\partial^2 z}{\partial x^2} - \frac{\partial^2 z}{\partial y^2} \right)^2}$$

- Saddle point $\kappa_1 \kappa_2 < 0$, extrema $\kappa_1 \kappa_2 > 0$
- Mean curvature which can be safely used in Hertz theory: $\bar{\kappa} = \sqrt{\kappa_1 \kappa_2}$

Asperity analysis







Rough surfaces and associated asperities

V.A. Yastrebov

Lecture 4

112/131

Asperity analysis



k_i=16, k_s=128, H=0.8





Rough surfaces and associated asperities

V.A. Yastrebov

Lecture 4

113/131

Asperity analysis





 Yastrebov et al, Three-level multi-scale modeling of electrical contacts sensitivity study and experimental validation, Proceedings of Holm Conference, 2015.



Asperity curvatures



 Yastrebov et al, Three-level multi-scale modeling of electrical contacts sensitivity study and experimental validation, Proceedings of Holm Conference, 2015.

Examples



in collaboration with A. Marchenko



Examples



In collaboration with D. Tkalich (NTNU, Sintef)





V.A. Yastrebov













■ Scale 4 (x100): PDF



What did you learn?

- Idea about the interface physics complexity
- How to measure roughness: confocal, WLI, AFM, STM
- What are the main characteristics: PDF, PSD, *S*_{*q*}, *S*_{*dq*}, Hurst, Nayak's parameter, etc
- Model roughness
- Fractal aspect & Mandelbrot set
- Real roughness

Thank you for your attention!

 \odot