nCATS

UNIVERSITY OF Southampton

Toward frictionless engineering surface

Tomáš Polcar

nCATS – Centre for Advanced Tribology, University of Southampton, UK

&

Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague

&

AdvaMat, s.r.o., Prague, Czech Republic

Tomas Polcar

Czech Technical University in Prague

Head of Advanced Materials Group
Full professor in Applied Physics

UNIVERSITY OF Southampton

Head of nCATS
Associate professor in Coatings and Nanotribology

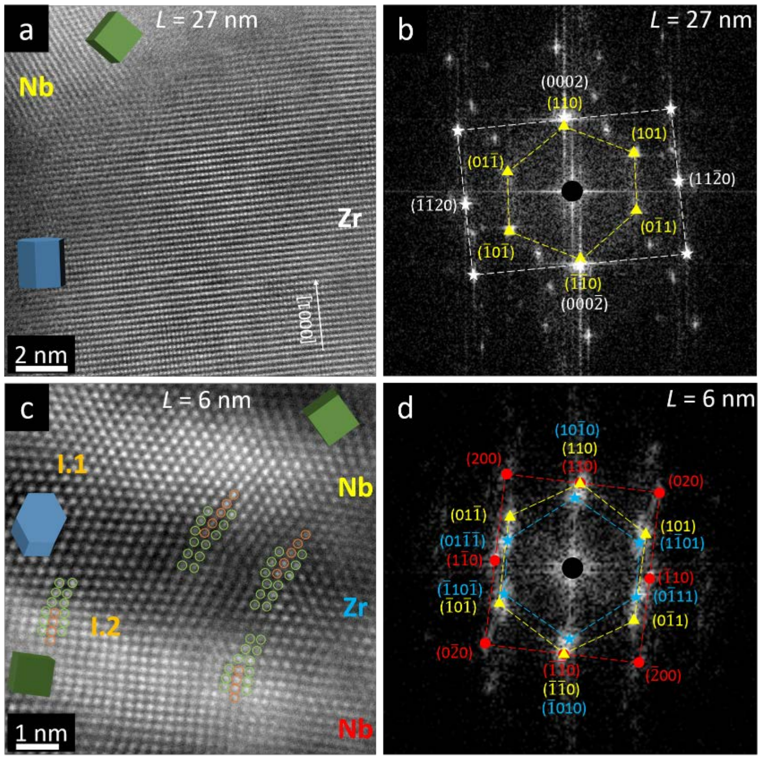
ADVAMAT

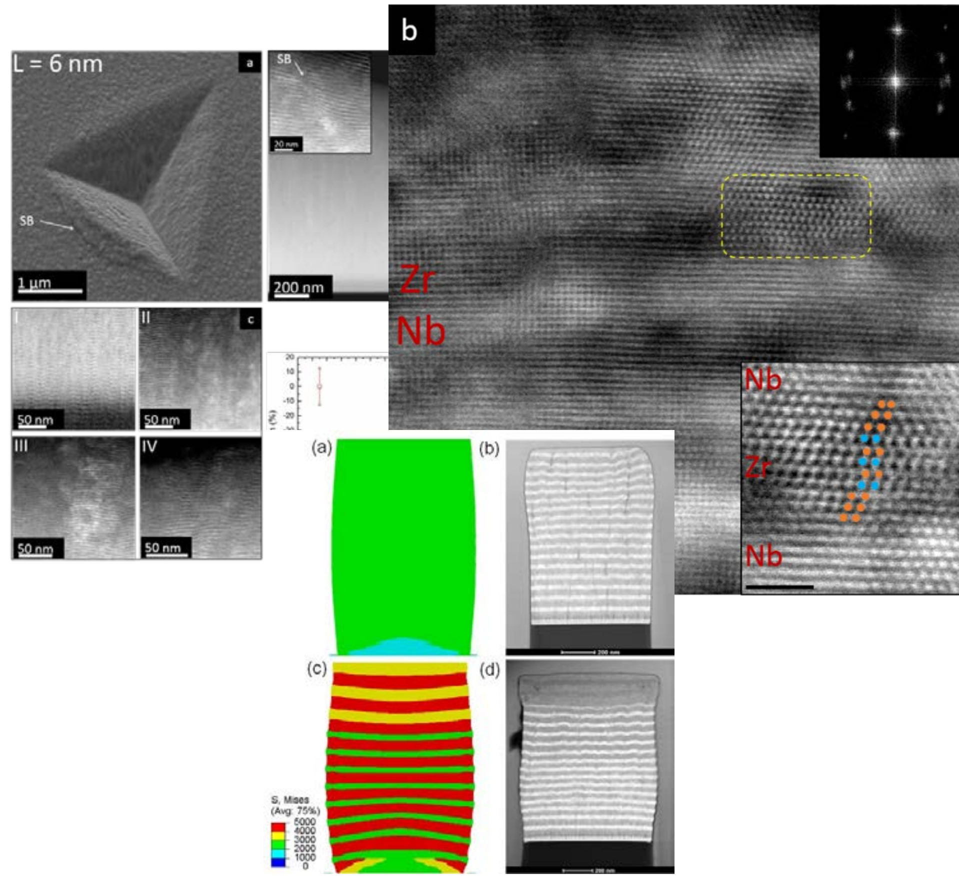
Spin-out company (Czech)
Coatings and material design
Owner

CEMUC

CEMUC – University of Coimbra
Visiting professor
Collaboration with A. Cavaleiro

Mechanical properties of Zr/Nb nanolayers

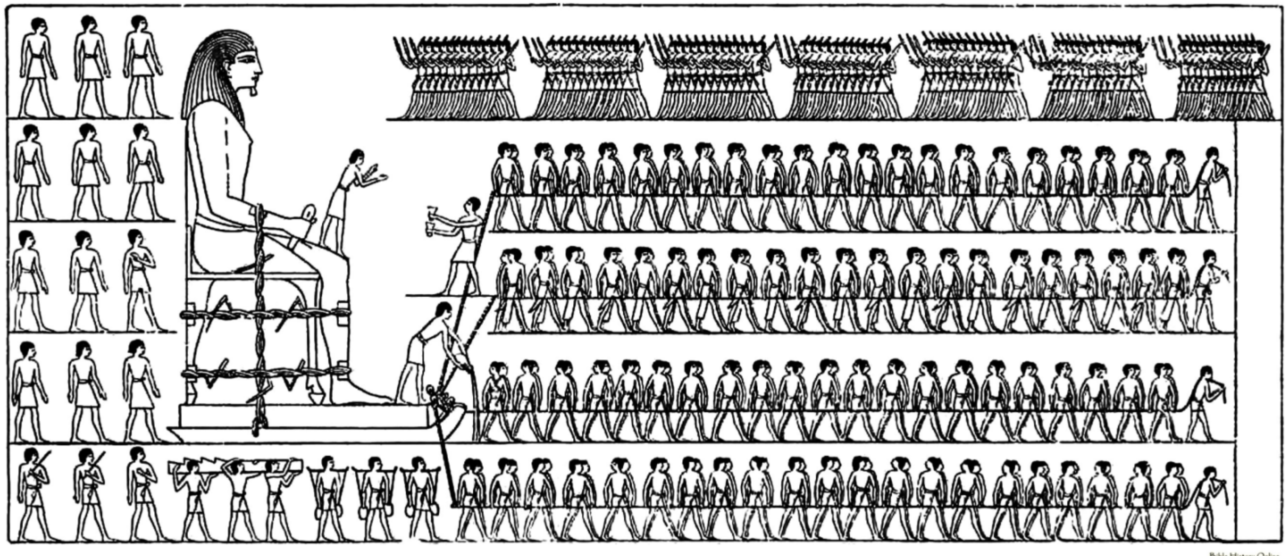




Monclus et al, Acta Materialia 2017
Callisti&Polcar, Acta Materialia 2017

Cool stuff? Yes, but for few of us!

Motivation I

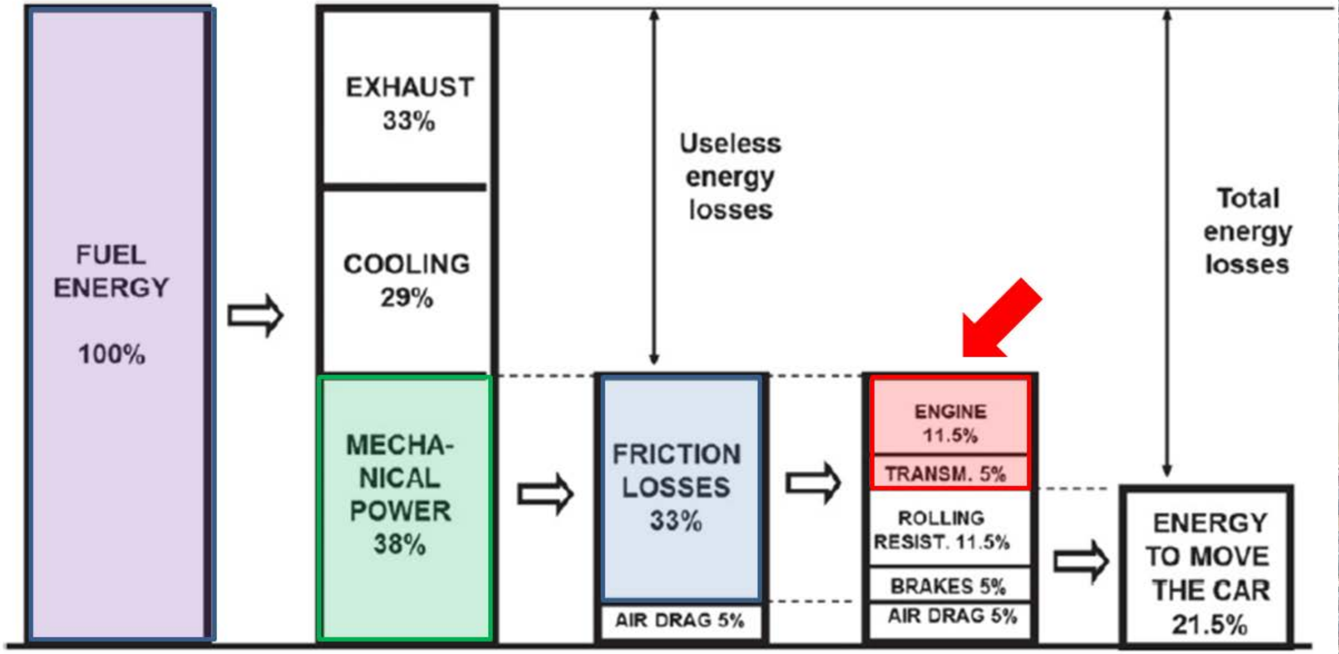


There are 162 men pulling approx. 60 ton statue.

“Tribologist” pour water to reduce friction from 0.3-0.5 (dry wood/wood) to 0.2 (wet wood).

Can I pull the statue alone?

Motivation II



- About 33% of fuel is wasted to overcome friction in passenger cars

- If friction losses are reduced 60%

…576,000 millions Euros

…385,000 millions liters of fuel

…960 millions tones of CO2 emission reduction

Holmberg et al, Tribology International 47 (2012) 221

Motivation III

Liquid lubrication (oils, greases) is:

- **most common in sliding applications**
- **very effective**
- **cheap**
- **decreasing friction and wear simultaneously**
- **reducing the temperature (cooling)**

However, there are significant disadvantages:

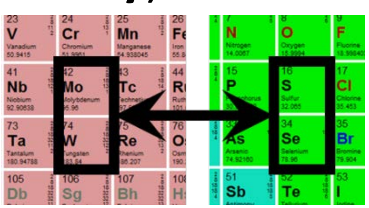
- **Use of non-renewable resources (over 40m tons globally per year)**
- **High energy-input for production**
- **Not really environmentally friendly**
- **Expensive maintenance**

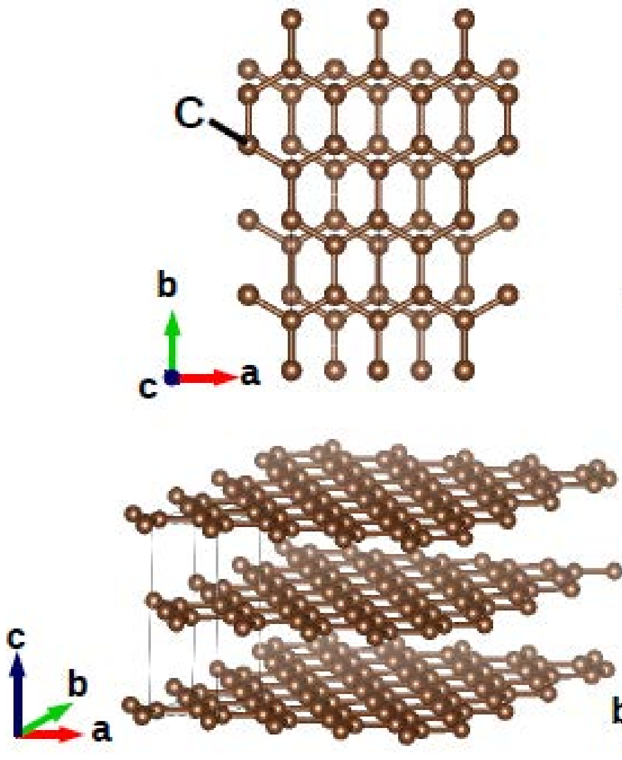
Can we replace them by solid lubrication?

Candidates for ultra-low friction solid lubricants

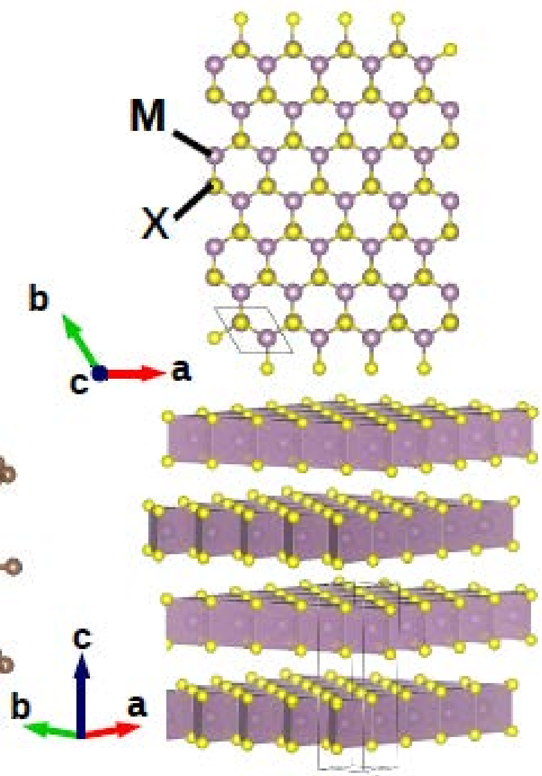
In mechanical engineering, solid material with friction coefficient < 0.1 is considered as a candidate for dry sliding applications.

There are many solid lubricants, but two of them emerge – carbon based materials (graphite/**graphene**) and transition metal dichalcogenides (**MoS_2 family**).





Graphene



MoS_2

nCATS

UNIVERSITY OF Southampton

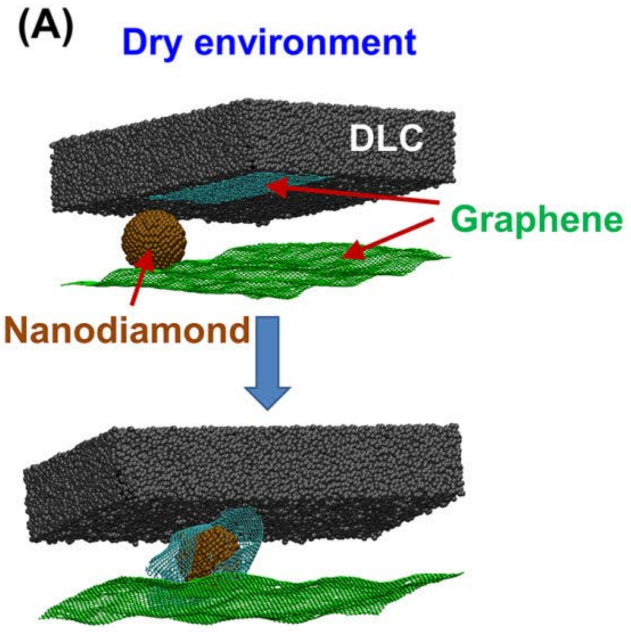
Candidates for ultra-low friction solid lubricants

What is the best material for dry sliding applications?

2D materials opens new horizons in tribology; previously unknown lubrication mechanisms could be harvest to minimize friction.

Graphene is the most studied material; however, its use in real industrial application is still very limited.

The major limitation of graphene is its nature – 2D material which must be forced into sliding interface…

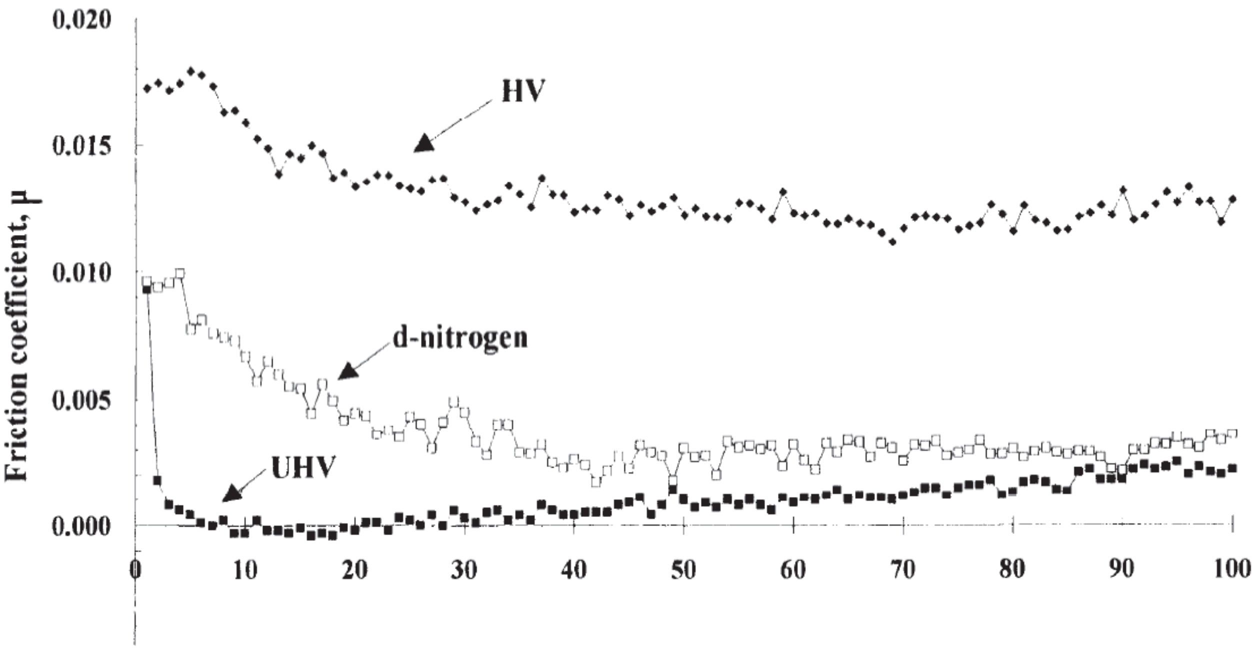


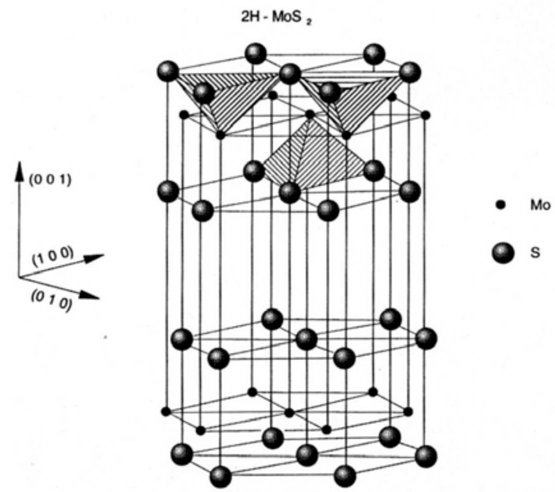
Berman D, Deshmukh SA, Sankaranarayanan SK, Erdemir A, Sumant AV, Science. 2015 5;348(6239):1118-22

Candidates for ultra-low friction solid lubricants

In ultra-high vacuum, MoS_2 crystal exhibited almost frictionless movement

However, the material is very sensitive to presence of water – friction is much higher





Transition metal dichalcogenides are versatile (self-assembly; chemical tailoring, etc.). Moreover, they exhibit decrease of friction with increasing load…

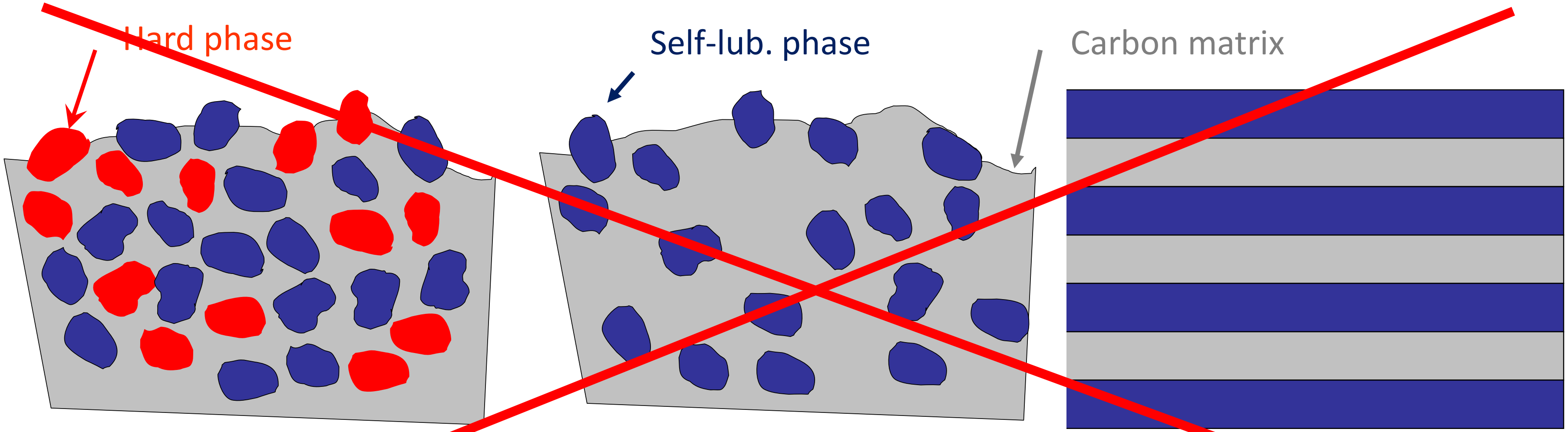
Martin et al Phys. Rev. B., 48 (1993) 14; Tribol. Int. 29 (1996) 123

How to design solid lubricant coating?

- Bulk solid lubricants are extremely soft…
  … we typically need hard surface.
- Solid lubricants are very sensitive to environmental attacks…
  … we want they work in different conditions.
- Wear rate of solid lubricants is very high…
  … we need high wear resistance (coating thickness 0.1-3 µm).
- Adhesion of solid lubricants is low…
  … we need that at the surfaces in contact.

→ Clearly it is very challenging to use them alone. We have to combine them to keep their advantages and minimize disadvantages.

Structural design solid lubricant coating?



Voevodin, A. A., O'Neill, J. P. and Zabinski, J. S. (1999). Surf. Coat. Technol., 116-119, 36

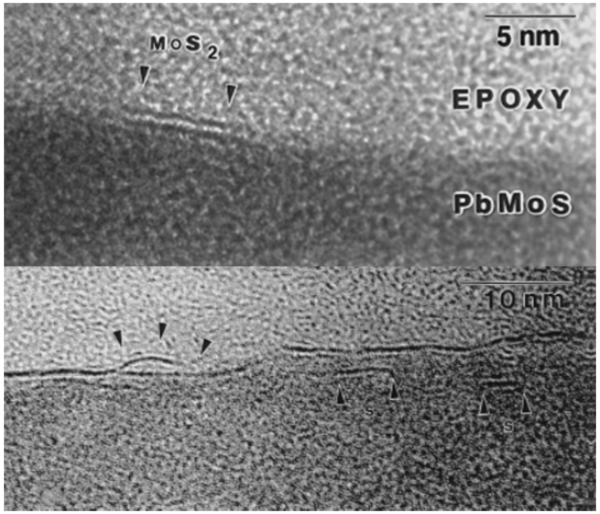
M. Evaristo, A. Nossa and A. Cavaleiro, Surf. Coat. Technol. 200 (2005) 1076.

J. Noshiro, S. Watanabe,T. Sakurai and S. Miyake, Surf. Coat. Technol. 200 (2006) 5849.

→ **Coatings prepared by magnetron sputtering**
→ **High wear, high oxidation rate, not that low friction…**

We need something better!

Do we need solid lubricant phase in as-deposited coating?

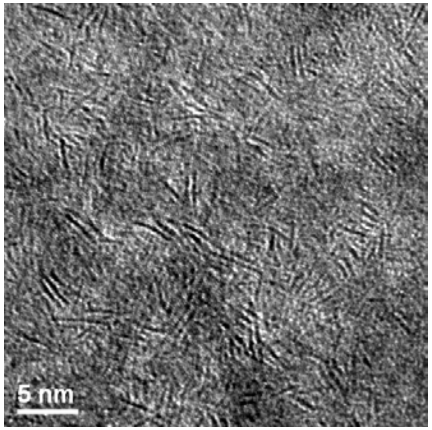


Sliding of amorphous Pb-Mo-S coating led to formation of crystalline MoS2 sheets
K.J. Wahl et al., Wear 1999

Apparently we do not need to have solid lubricant phase before sliding process; the combination of **shear stress and high contact pressure forms thin tribolayer** at the interface reducing friction.

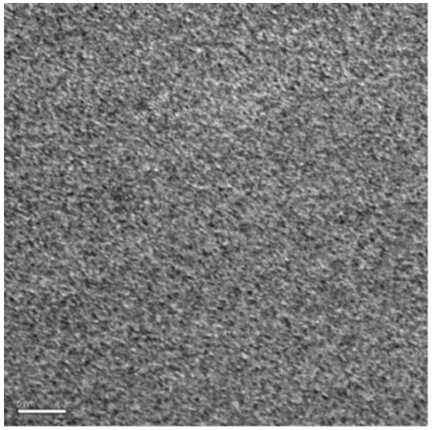
We prepared:

W-S-C



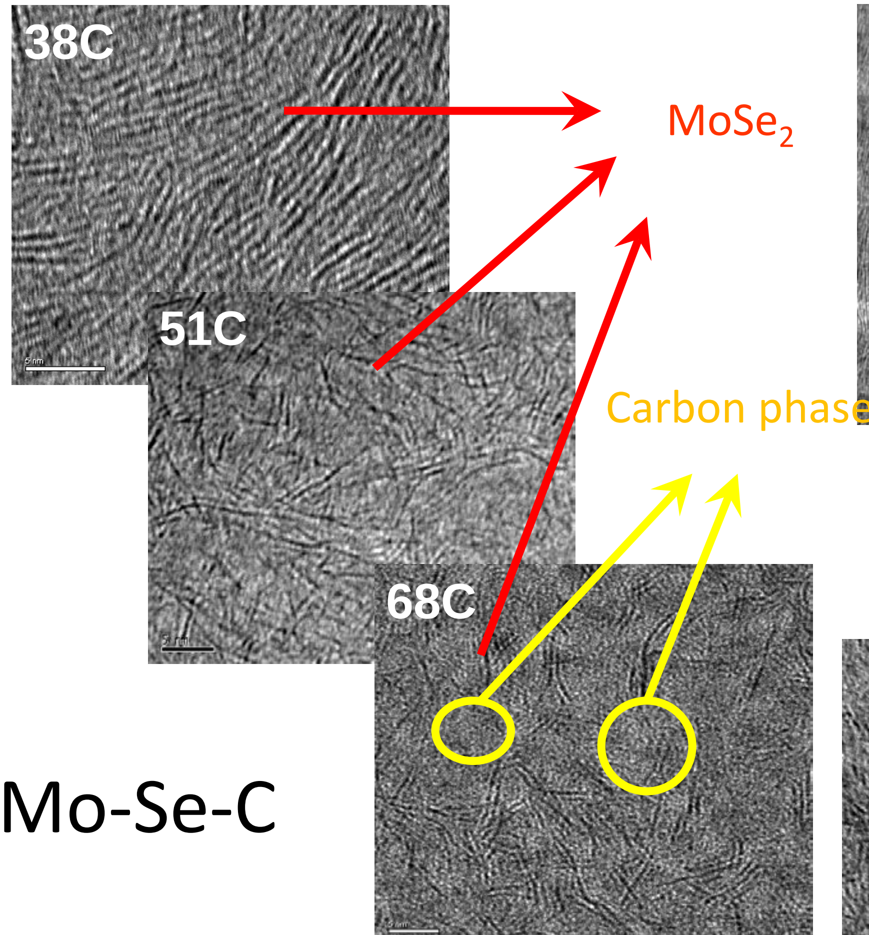
Nanostructured

W-S-N



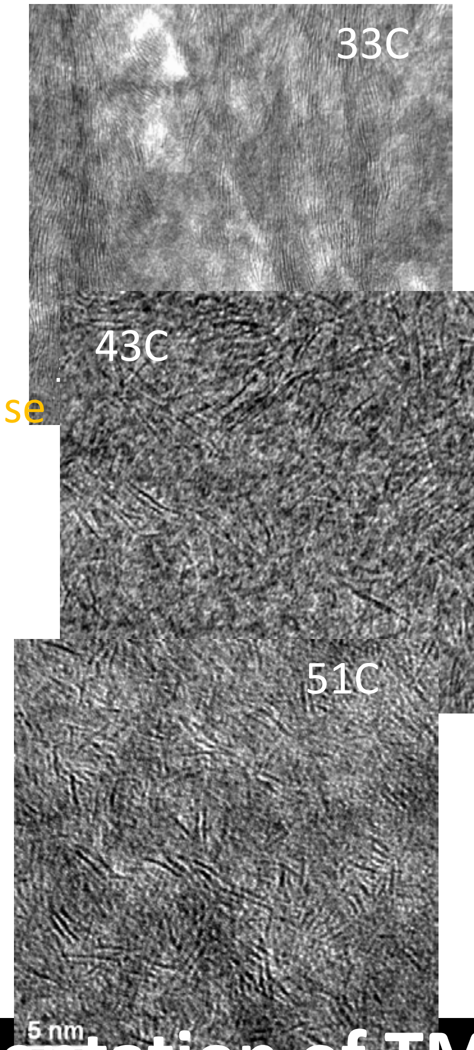
Amorphous

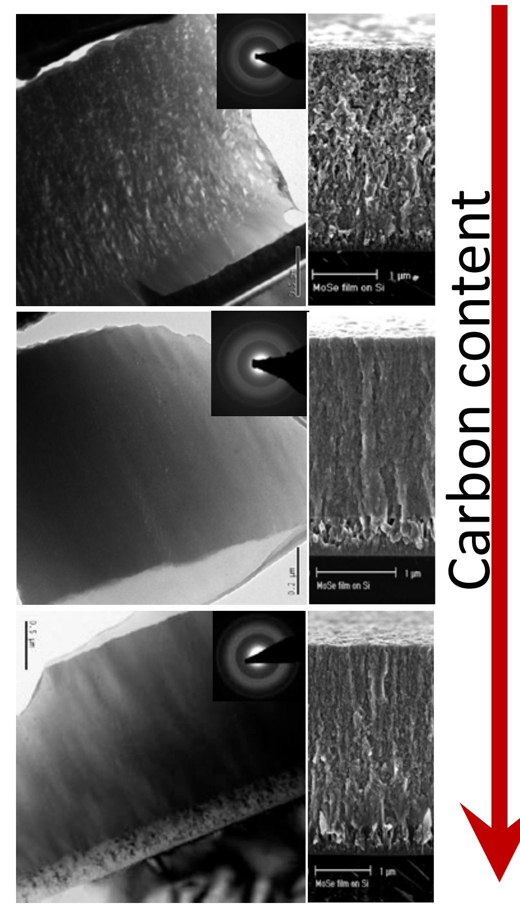
TMD – C films: microstructure



Mo-Se-C

W-S-C

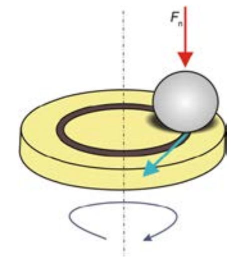




C. Sandu et al, Microscopy and Microanalysis 14 s3 (2008) 7;
T. Polcar et al, Plasma Processes&Polymers, 2009, 6, 417

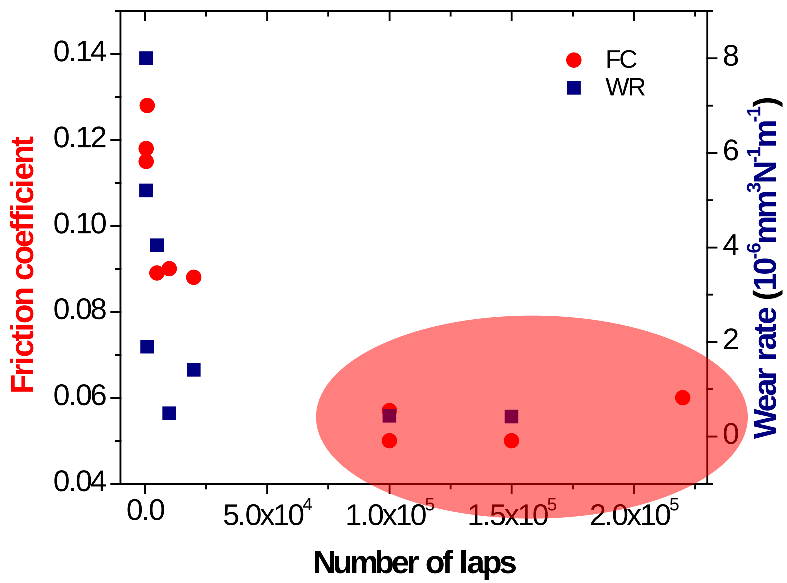
Random orientation of TMD platelets

Tribology: Extremely high loads and long running-in

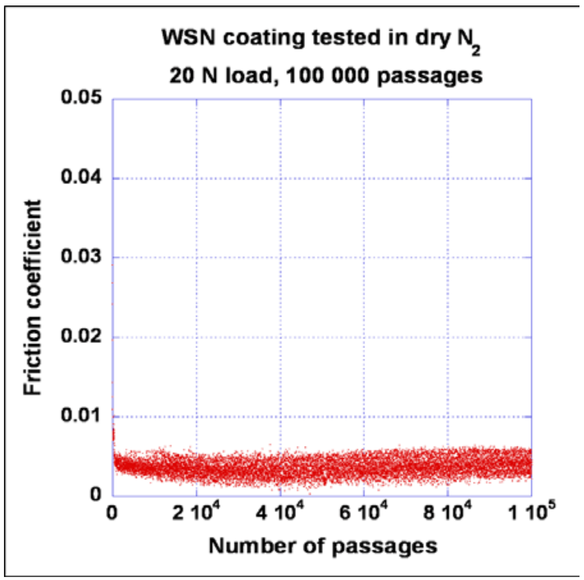


Reciprocating ball-on-disk**; 100Cr6 Ball**

WSC film – sliding in humid air

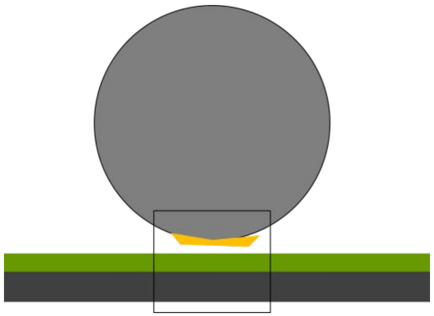


WSN film – sliding in N2

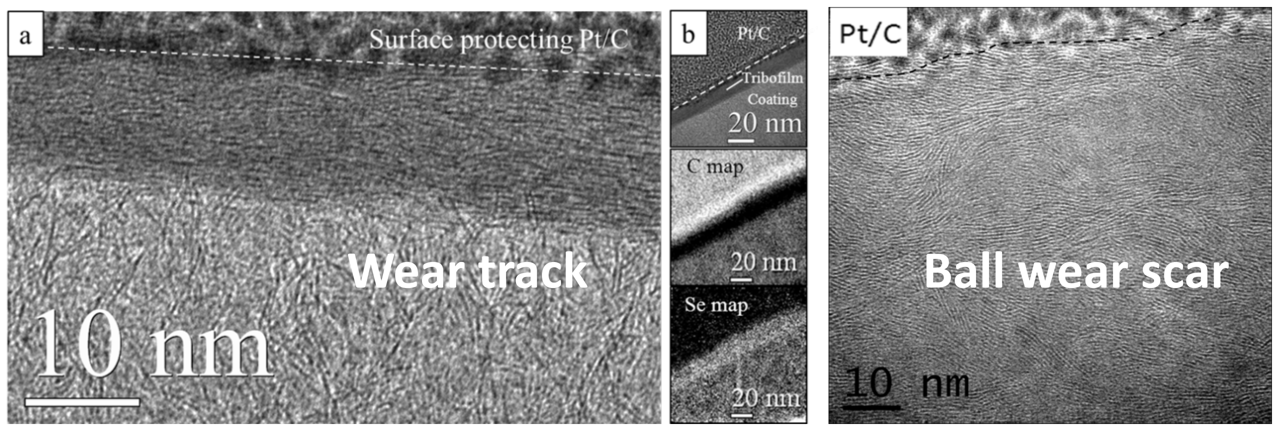


Polcar et al, Wear 266 (2009) 393; Polcar et al, Wear 266 (2009) 388;
Pimentel et al, Surf Coat Technol 205 (2011) 3274; Pimentel et al, Tribol Int 47 (2012) 188

Analysis of the wear track – FIB/TEM & AES

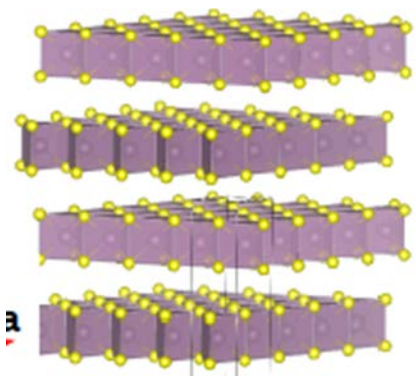


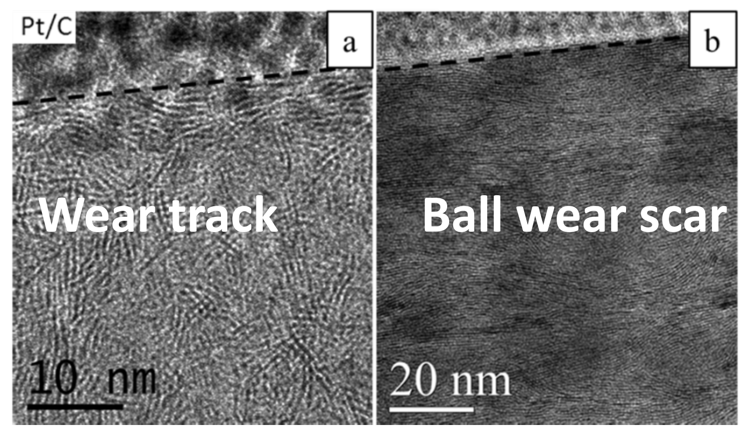
Humid air



Nitrogen

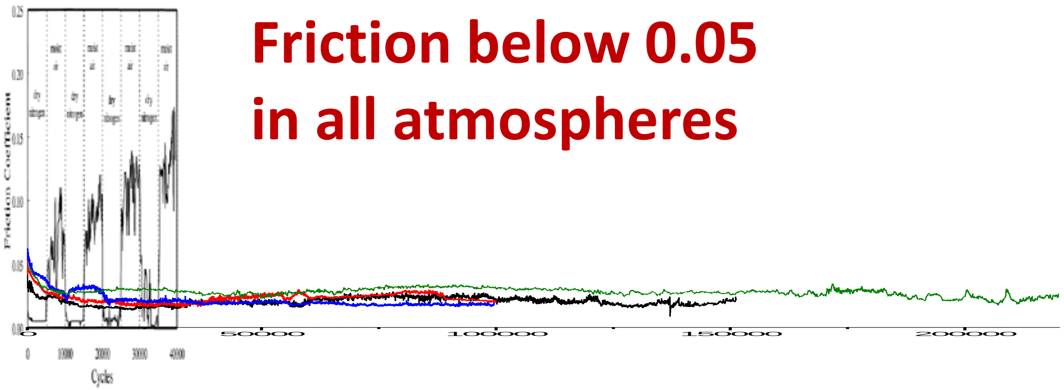
Well ordered thin TMD tribolayer formed at sliding interface



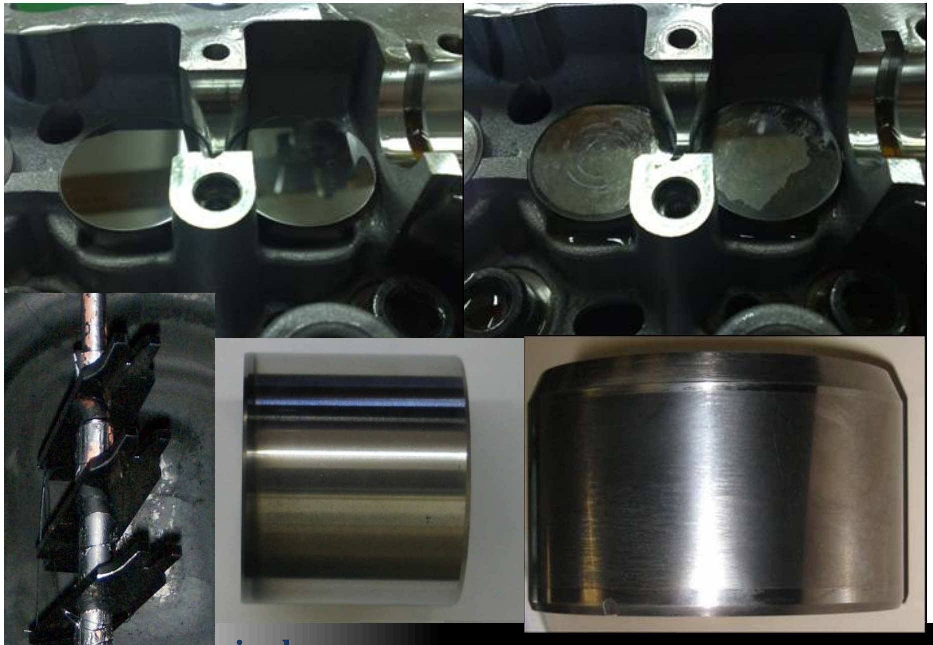


Polcar et al, Faraday Discussions 2012; Gustavsson et al, Surf Coat Technol 2013; Gustavsson et al, Wear 2013; Gustavsson et al, Trib Trans 2015

Does it really work?



Friction below 0.05 in all atmospheres



WSC coating were successfully up-scaled and deposited on real 3D parts

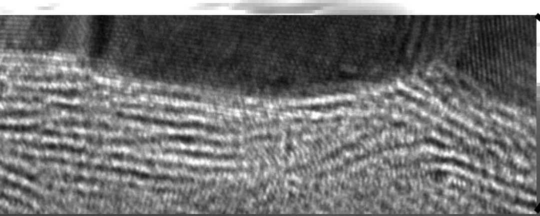
The coatings were tested by several companies in various applications:
→ Vacuum bearing
→ Automotive engine
→ Tools

Results were in general very positive…

Final concept (?)

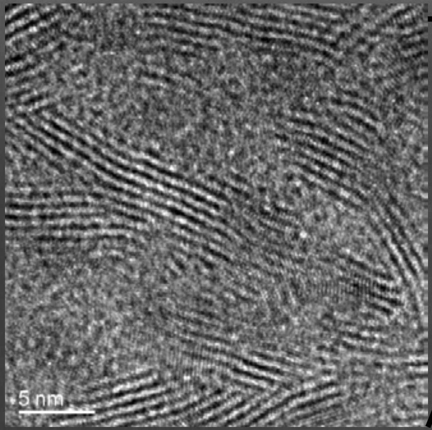
Carbon worn out immediately (mostly in graphitic form)

Tribolayer with 002 TMD phase



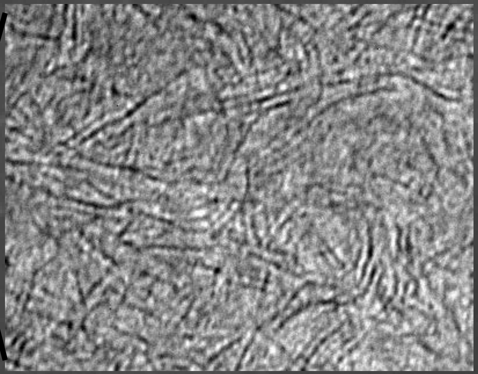
- Low fiction
- Minimal oxidation
- No voids or cracks

Sub-surface adapted layer



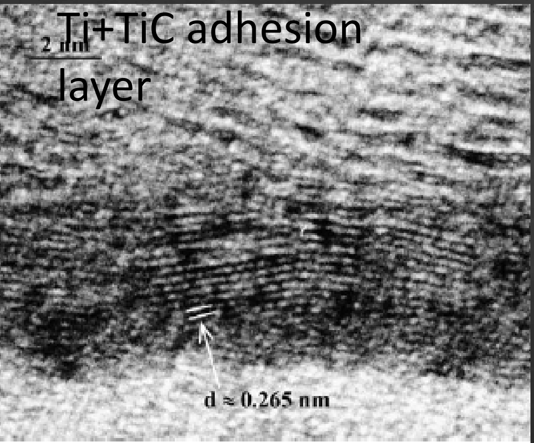
- Re-oriented TMD platelets
- Improved mechanical properties (H increases)
- High density

As-deposited coating



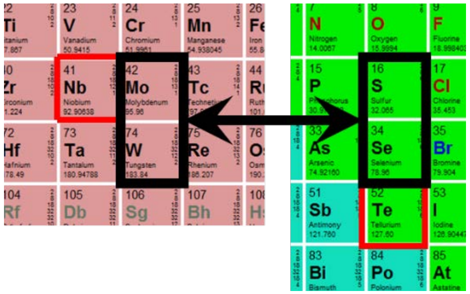
- Structure with easy self-adaptation

Ti+TiC adhesion layer



End of story? No!

- There are 4 members of transition metal dichalcogenides family
  - which one the best candidate for specific application?



- Friction decreases with contact pressure.
  - why?
- Environmental sensitivity
  - detrimental effect of water?
- Relation between nanoscale models and experiments with macroscale tribology.
  - can we replicate macroscale measurement at nanoscale?

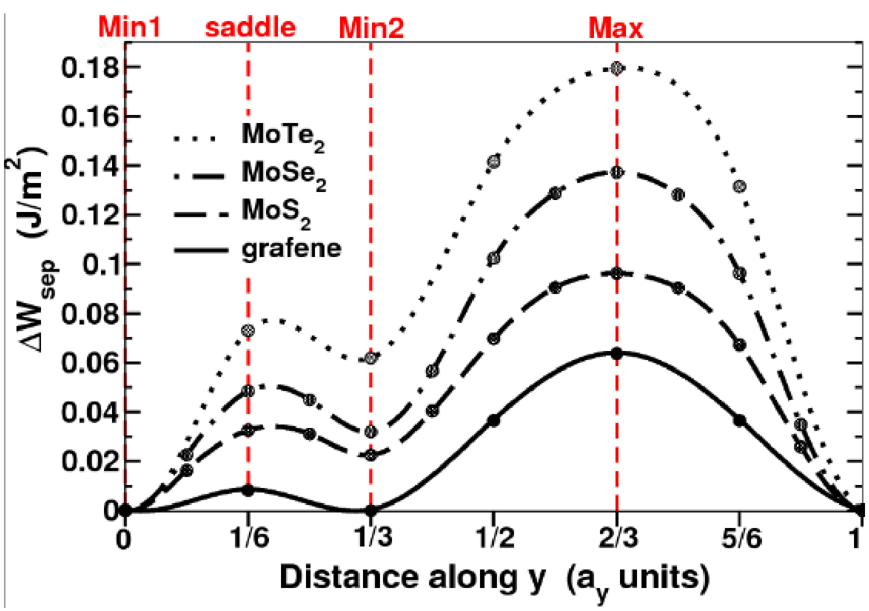
To answer these questions, multiscale simulations with tailored experiments are needed!

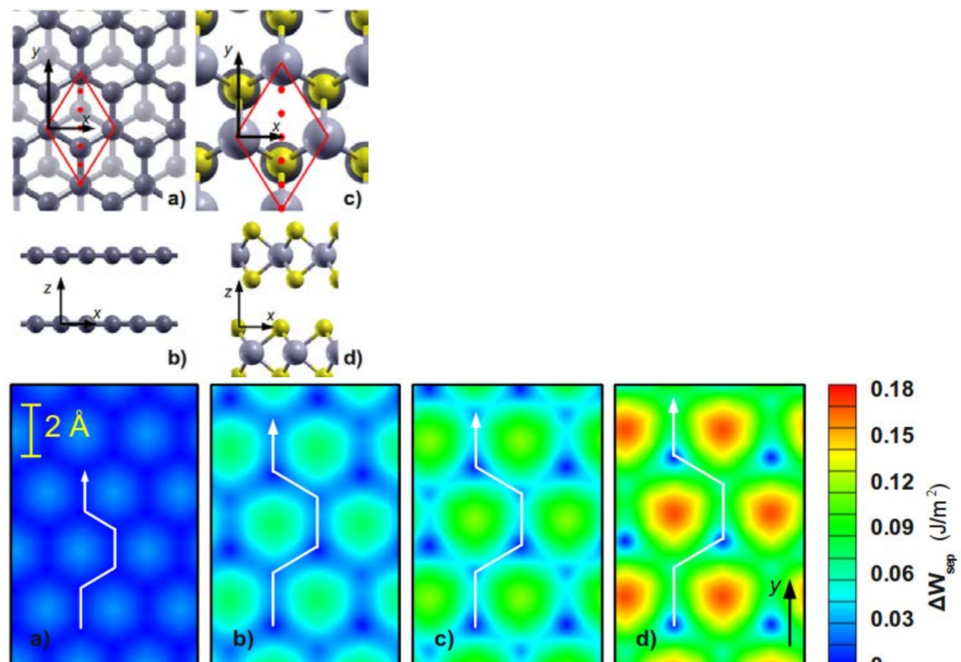
Bottom-up approach: ab initio

Frictional properties of ideal bulk TMD crystal (in engineering terms: which TMD does exhibit the lowest friction?).

Ab initio – potential energy landscape.

Collaboration with G. Levita& M.C. Righi: Load and orientation effect on friction



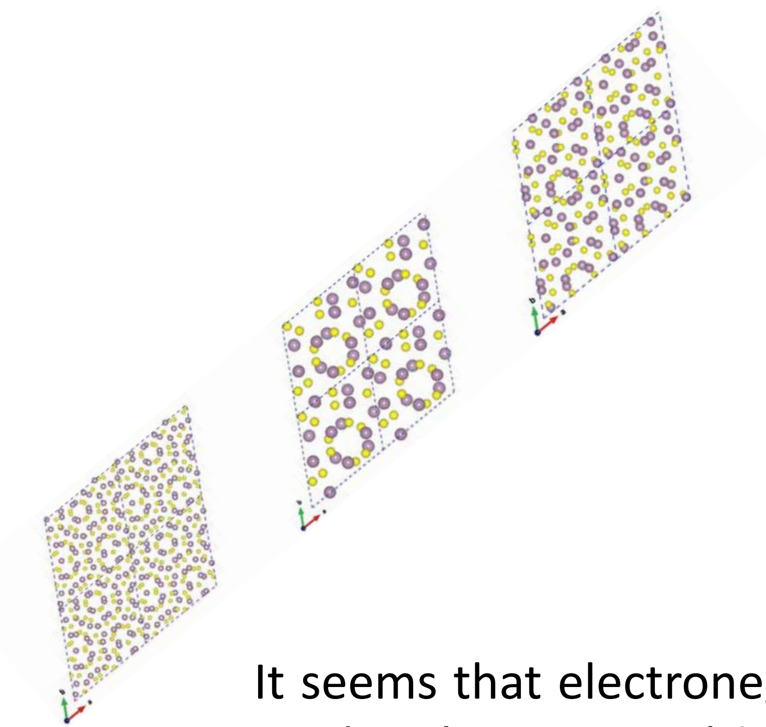


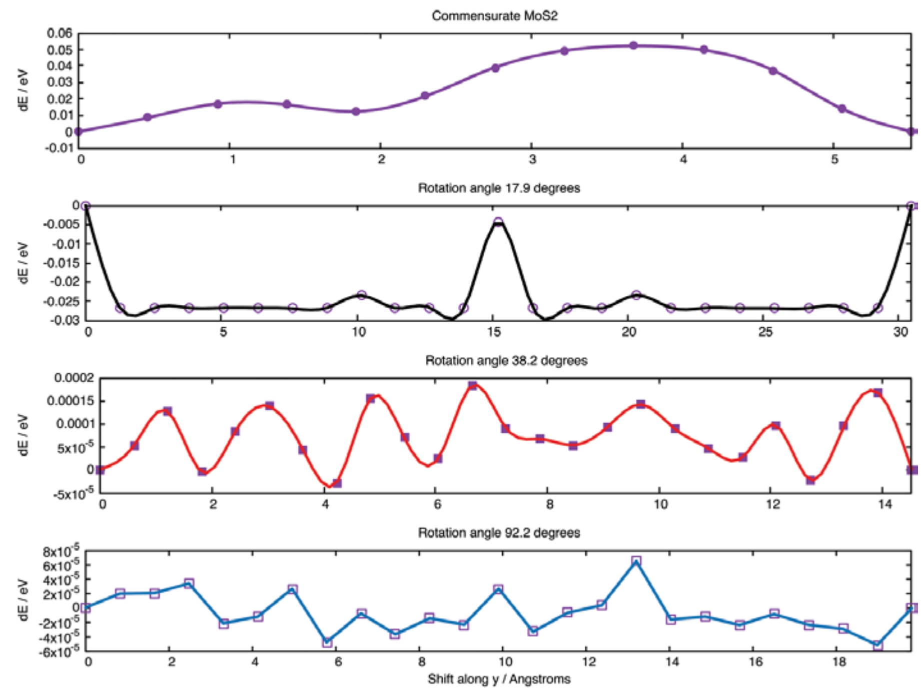
Graphene MoS2 MoSe2 MoTe2

G. Levita et al, J Phys Chem C 2014; G. Levita, E. Molinari, T. Polcar, M.C. Righi, Phys Rev B 2015

Bottom-up approach: ab initio

We can now use PES to explore intrinsic friction commensurate surfaces… However, it is the highest energy barrier for slip. We need to check incommensurate surfaces too!





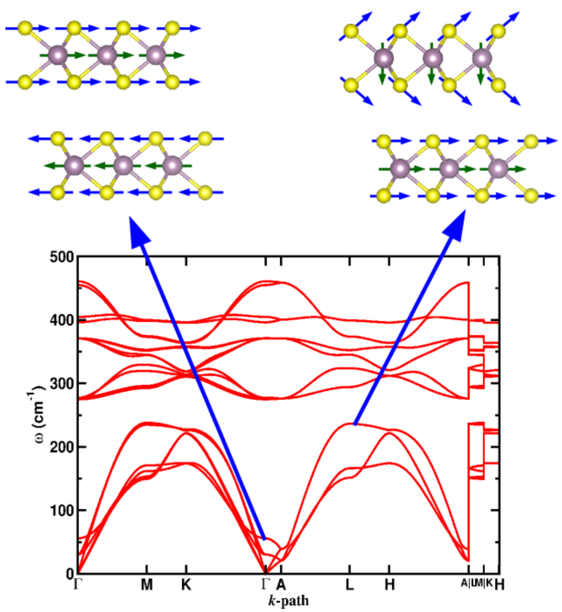
It seems that electronegativity could be used as a simplified parameter to predict shear strength!

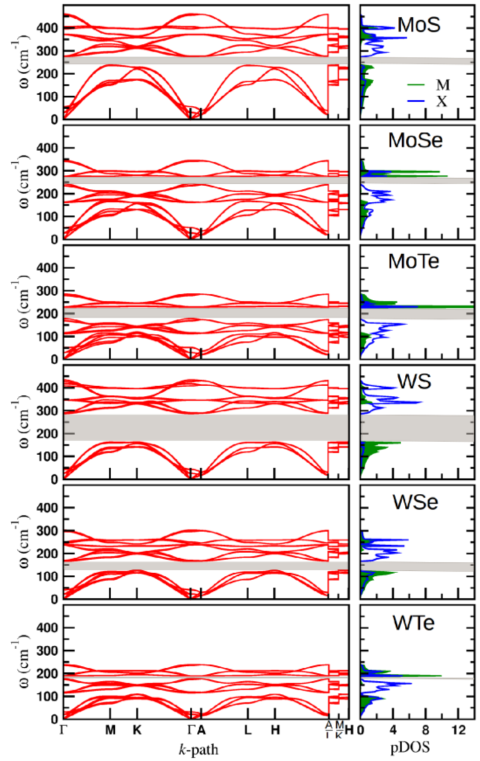
B. Irving, P. Nicolini, T. Polcar, Nanoscale 9 (2017) 5597

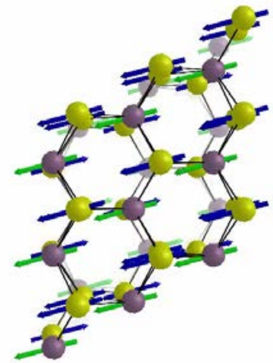
Bottom-up approach: ab initio

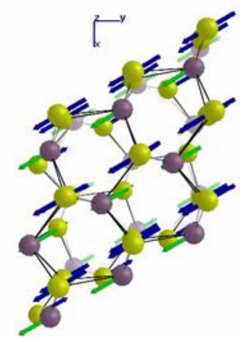
Ab initio –vibrational frequencies of the distortion modes.

Let’s ***assume*** the friction is related to vibrational frequencies of Me-X pairs









A. Cammarata, T. Polcar, Inorganic Chemistry 2015

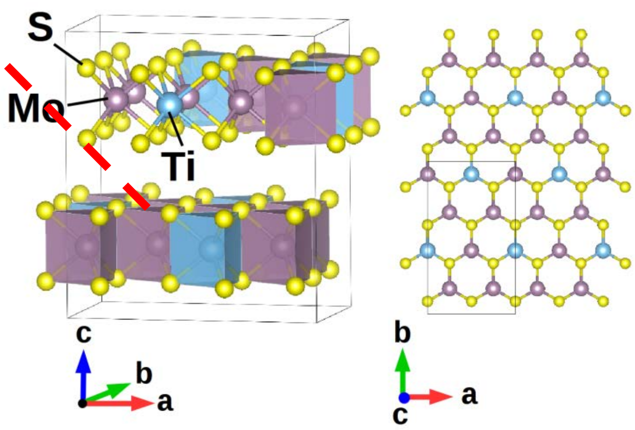
Bottom-up approach: ab initio

Sliding-relevant frequencies are stoichiometry-dependent (i.e. they depends on Me-X bond covalency):

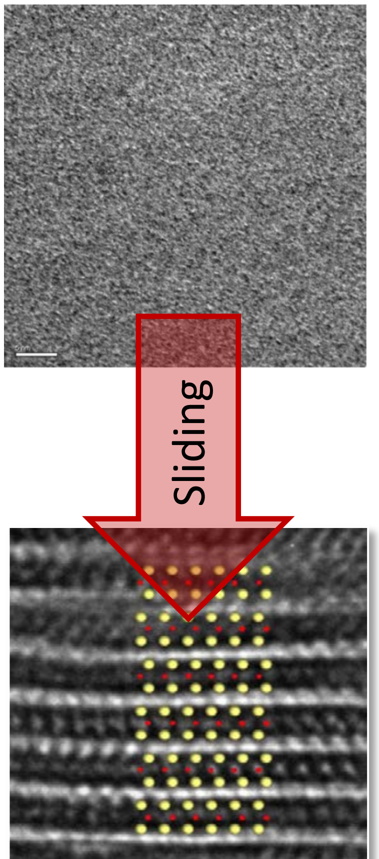
MoS_2 > $MoTe_2$ > $MoSe_2$ > WS_2 > WSe_2 > WTe_2

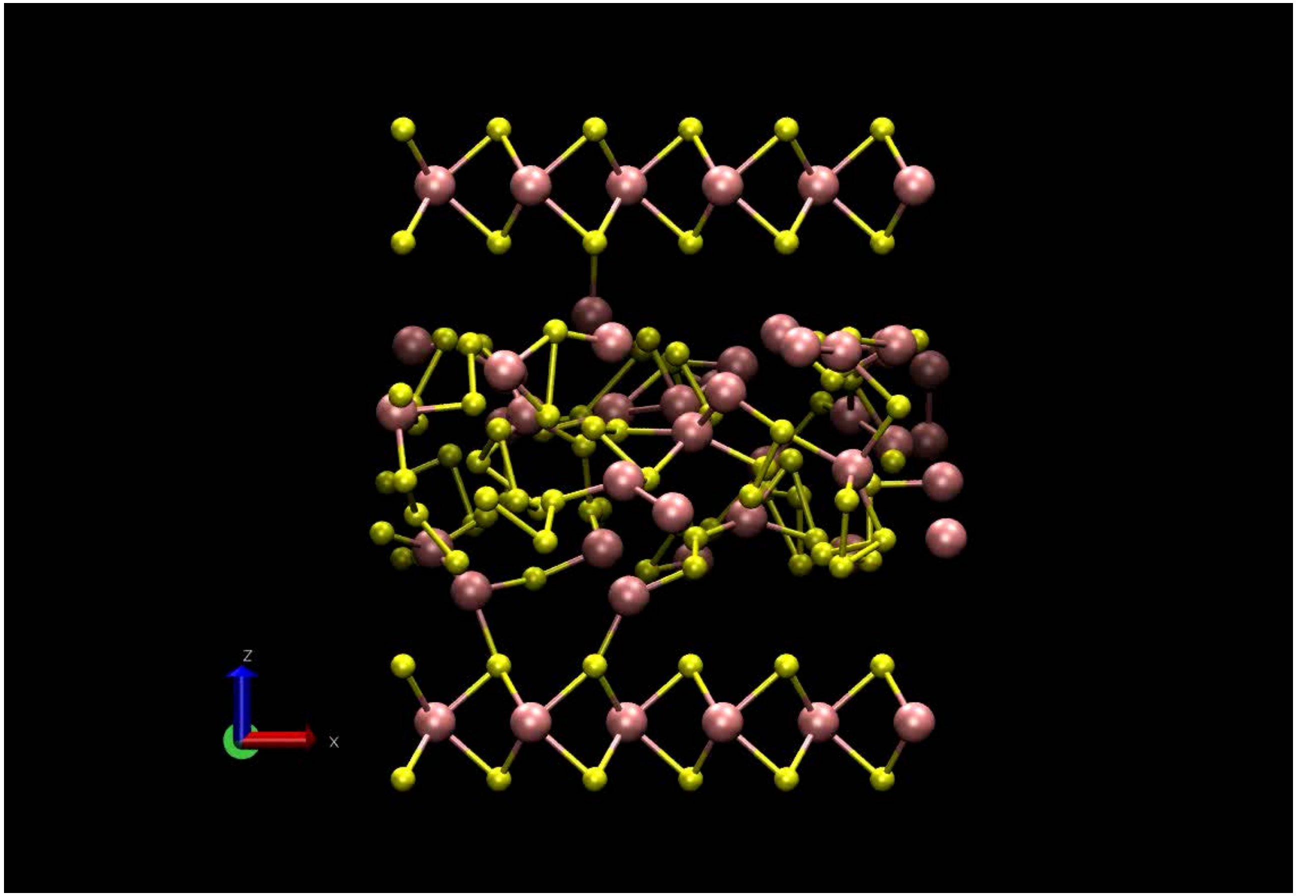
Therefore, assuming the friction is related to vibrational frequencies of Me-X pairs we can conclude that intrinsic friction follow the same trend.

We can use the same method to design new materials with low frequencies: MoS_2 doped with Ti



Formation of low friction layer

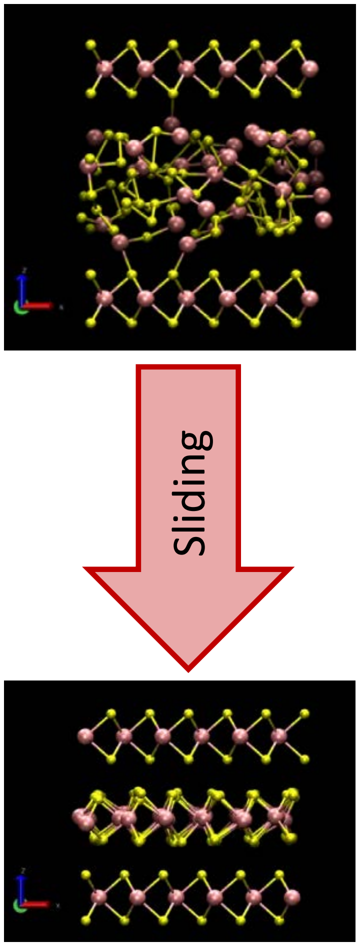




We are improving potential for MoS_2 (not perfect yet, but best to date) and use it to simulate sliding of quasi-amorphous MoS_2 between oriented MoS_2 layers

P. Nicolini, T. Polcar, unpublished

Formation of tribolayer – need for rough surface?



We have found that transformation from amorphous to crystalline MoS_2 is triggered by flash increase in temperature. This increase must be of short duration only (basically we can control it by termostat).

Is it somehow related to flash temperature during asperity contact?

Experiments suggest that:

- Higher contact pressure → quicker formation of tribolayer
- Higher temperature → quicker formation of tribolayer
- Sliding in oil → no tribolayer observed

P. Nicolini, T. Polcar, unpublished

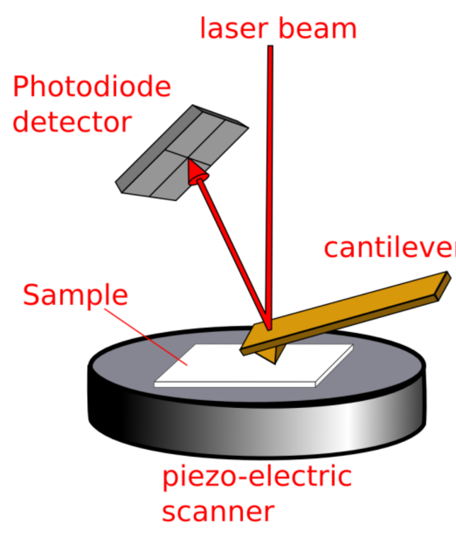
Simulations vs reality

An initio (Density Functional Theory) can treat few atoms (tens, hundreds) – extremely computationally demanding.

Molecular dynamics (classical or quantum) can simulate the systems with thousands to millions atoms.

The contact area of two hairs is approx. 200 billion atoms – more then starts in Milky Way…

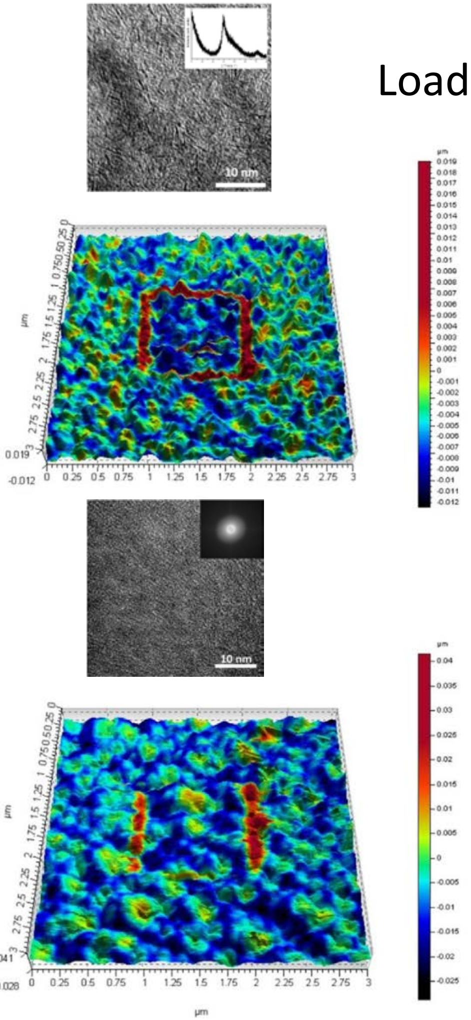
We need to find bridge between macroscopic sliding test and nanoscale simulations.



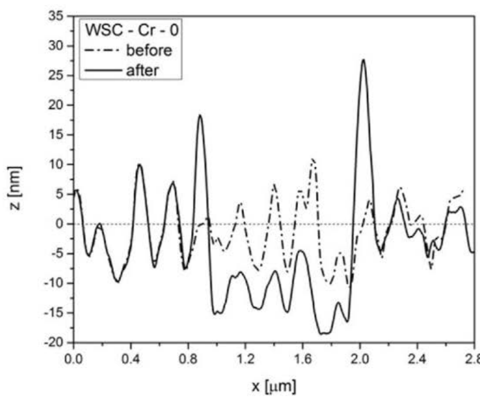
Atomic Force Microscopy

Macroscale vs nanoscale tribology

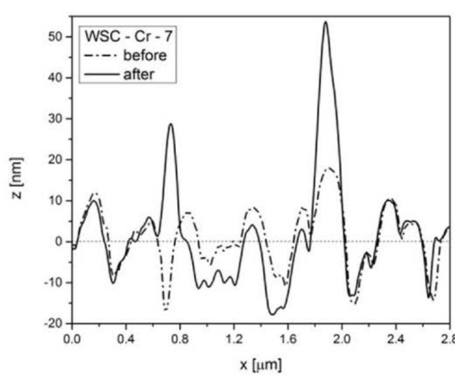
Load 100 nN; WSC/Cr coatings



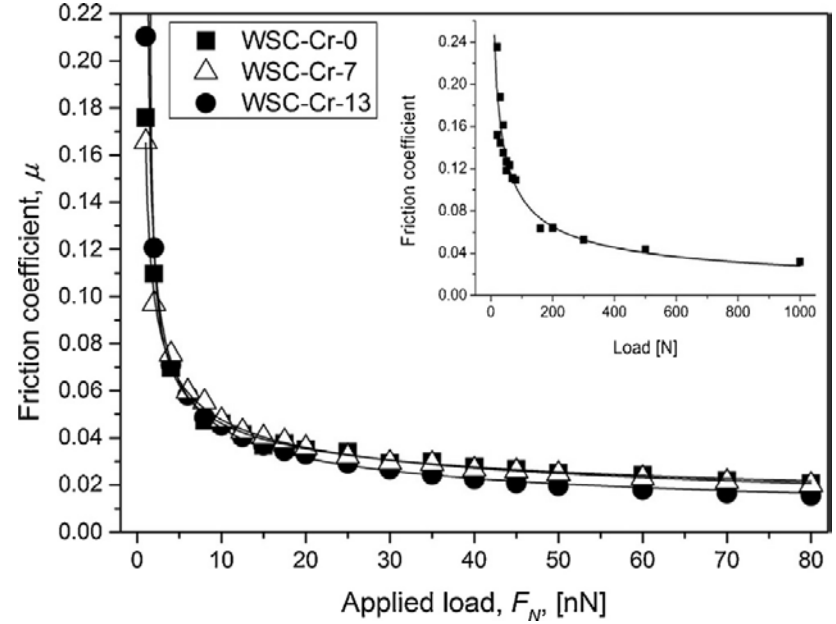
(c)



(b)



(d)

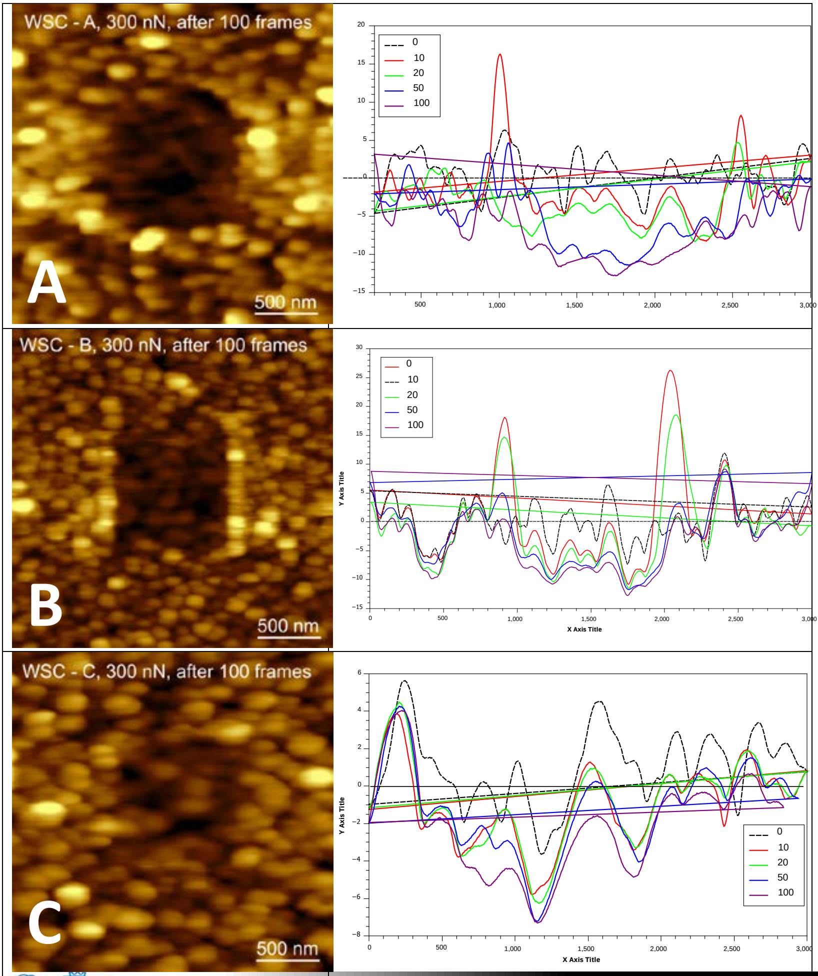


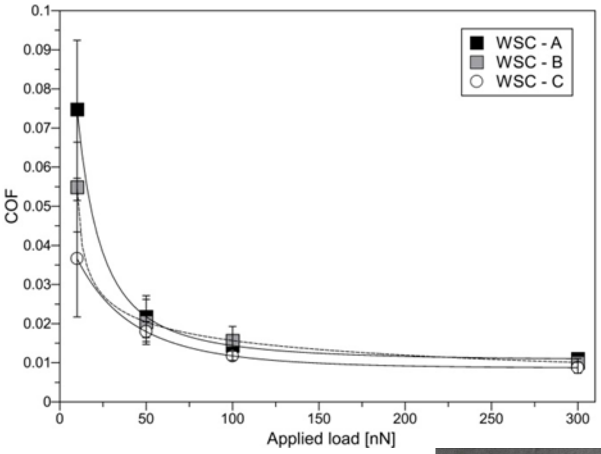
Friction coefficient follows the same trend. Note that contact pressure is similar in both sliding experiments

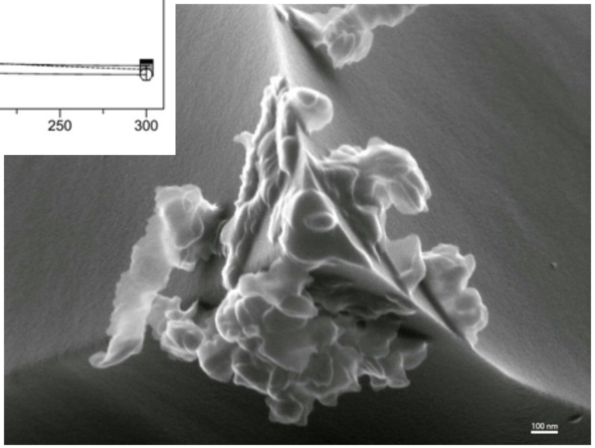
J. Zekonyte, T. Polcar, Appl Surf Sci, 2015

Macroscale vs nanoscale tribology

Load 300 nN; WSC coatings







Friction and wear trends replicate macroscale tests

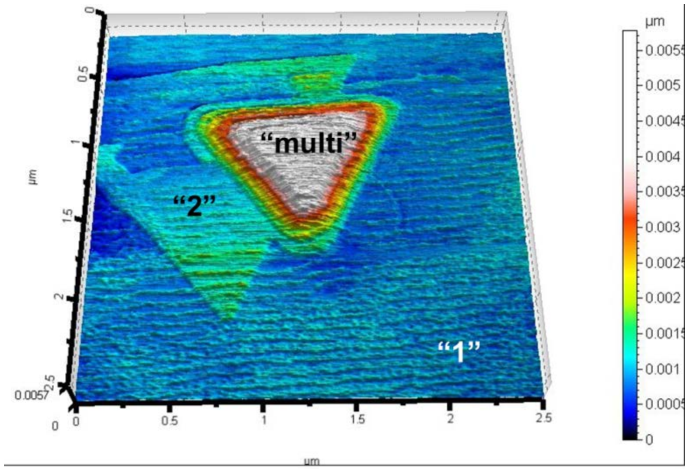
→ Wear is layer-by-layer; thin WS_2 sheets formed

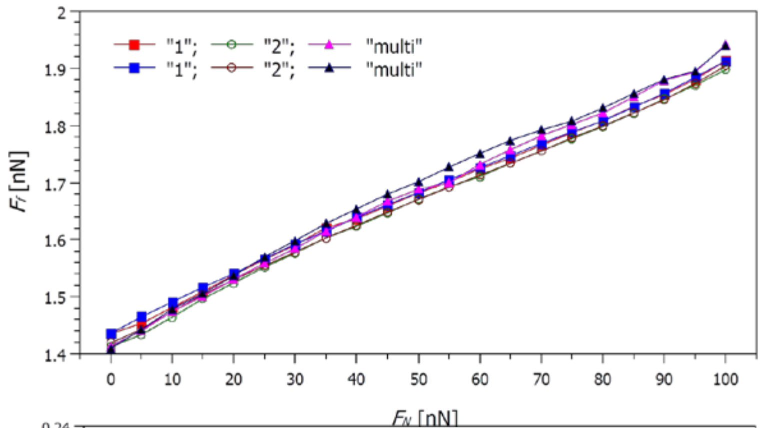
→ Very thin films should be functional as well

J. Zekonyte, T. Polcar, ACS Applied Materials & Interfaces, 2015

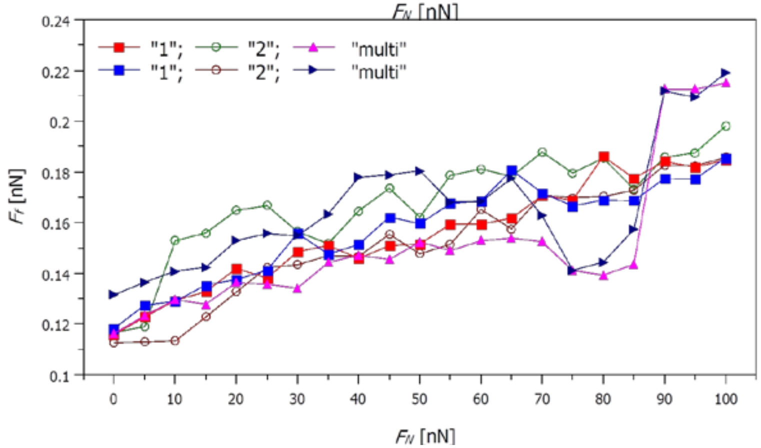
2D TMD sheet sliding: friction vs load

Investigation of sliding properties of 2D mono and multilayered WSe_2 system (collaboration with Lain-Jong Li from KAUST).





Si AFM tip



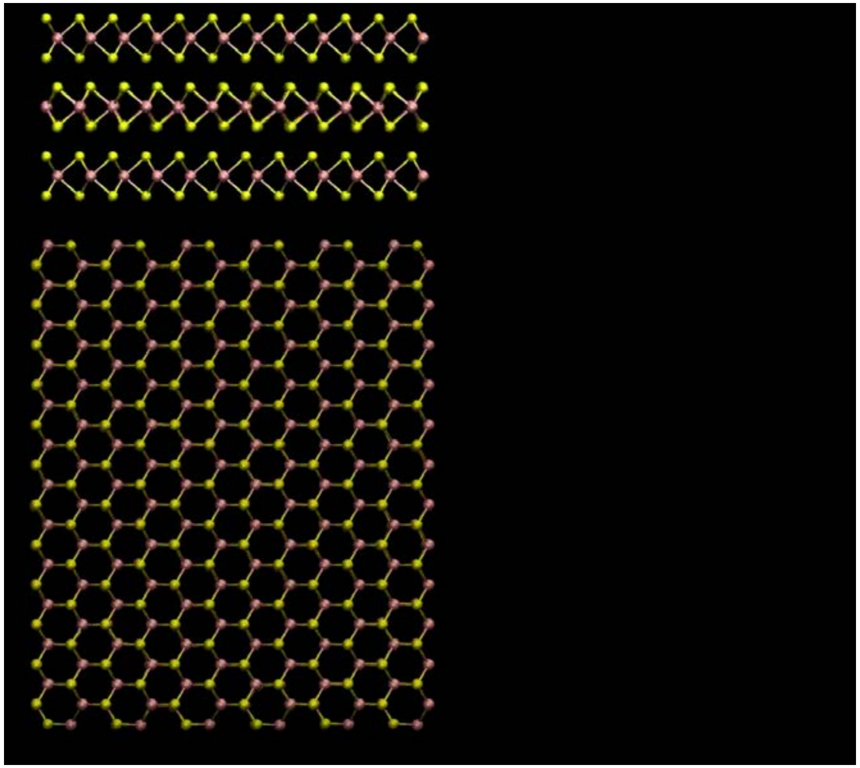
WSe_2 coated Si AFM tip

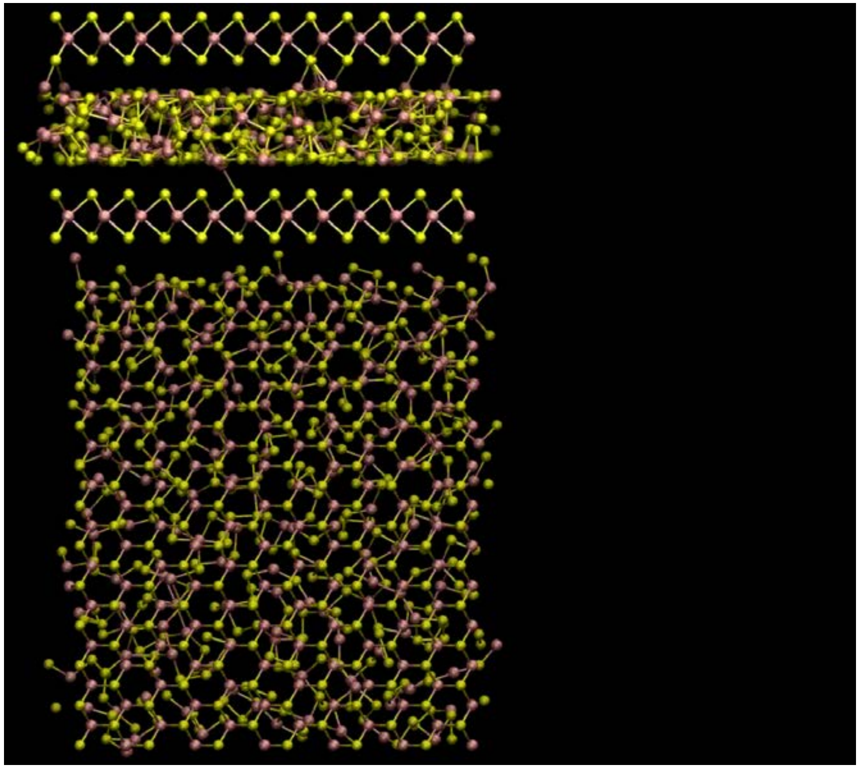
We have not observed any change in friction in 0-100 nN range – it seems that WSe_2 is Amontonian material…

Molecular dynamics: Effect of load

Increasing load (1 MPa – 10 GPa) tested on crystalline and amorphous MoS_2

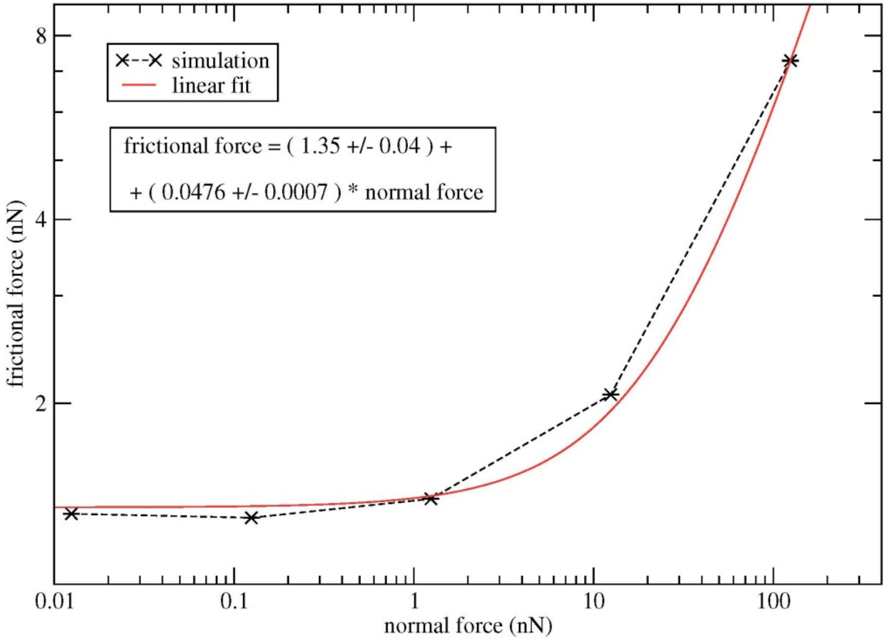
AIREBO force field [T. Liang et al., Phys. Rev. B, 79, 245110 (2009); Phys. Rev. B, 85, 199903(E) (2012)] using the LAMMPS package [S. Plimpton, J. Comp. Phys., 117, 1 (1995)].

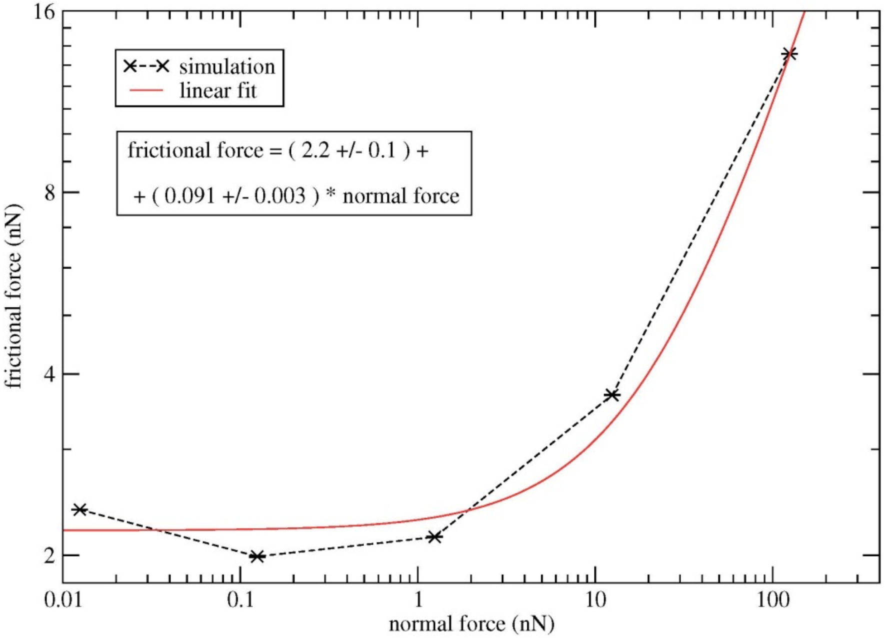




Molecular dynamics: Effect of load

Both crystalline (left) and amorphous (right) MoS_2 show perfect Amontonian friction (linear increase of frictional force with normal load).

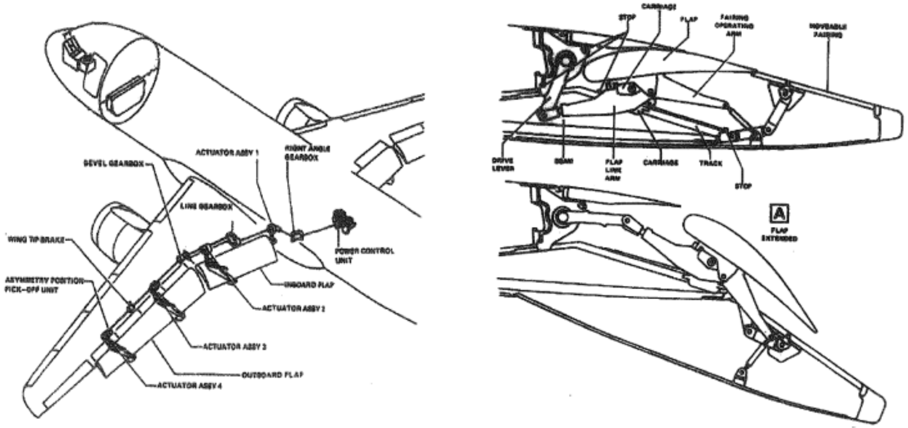




$$F_f = F_0 + \mu L$$

As expected, friction of amorphous MoS_2 is much higher than that of crystalline.

Industrial applications



Flap System Link-Track Flap Mechanism
(Airbus A320 Flap)

Gas sealing

Rifle scopes

You can save over 100 kg by using distributed electrical motors plus “dry” gear

14 PhD studentships (salary €3.0 – €3.9k) available right now!

Design strategy