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Metal-based Nanocomposites: Tribological Behavior Analysis through Atomistic Simulations

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Classification of Engineering Materials

In terms of MSE, materials are divided into three main categories: metals, ceramics and polymers

Metals

- High strength
- Electrical conductivity
- Thermal conductivity
- Flexible
- High weight
- Low resistance to corrosion

Composites

Polymers

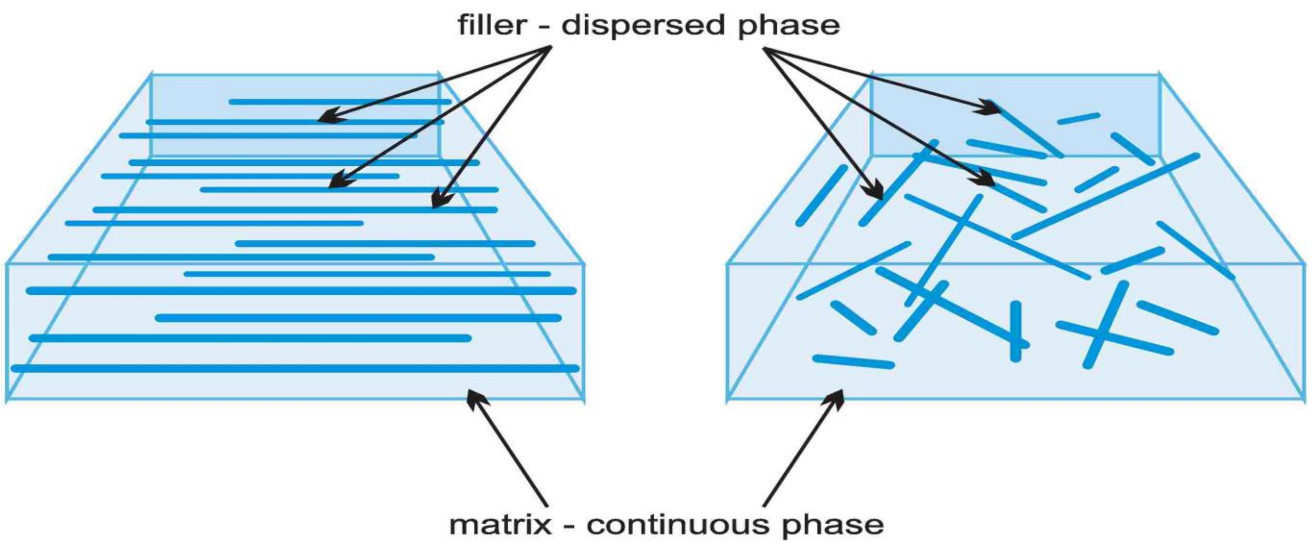
- Low weight
- Hight resistance to corrosion
- Flexible
- Electrical insulation
- Low strength
- Low resistance to heat

Ceramics

- High resistance to wear
- Electrical insulation
- Thermal insulation
- High strength
- Brittle
- High weight

What is composite?

Composite materials are engineered materials made from two or more constituents that remain separate and distinct while forming a single component.



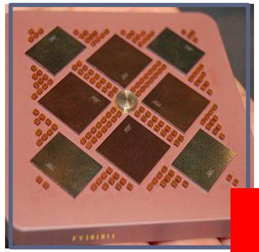
If the second phase is in the nanometer scale
i.e. <100nm
we will have a nanocomposite!

Why Metal Matrix Nanocomposites (MMNCs)?

- Better resistance to wear & corrosion
- Higher strength
- More Accessible
- Reduced coefficient of friction
- Lighter weight
- More Recyclable

Metal Matrix NanoComposites (MMNCs)
in comparison with conventional metals

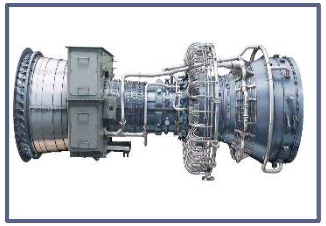
Applications of MMNCs



Electronic chipsets

Medicine

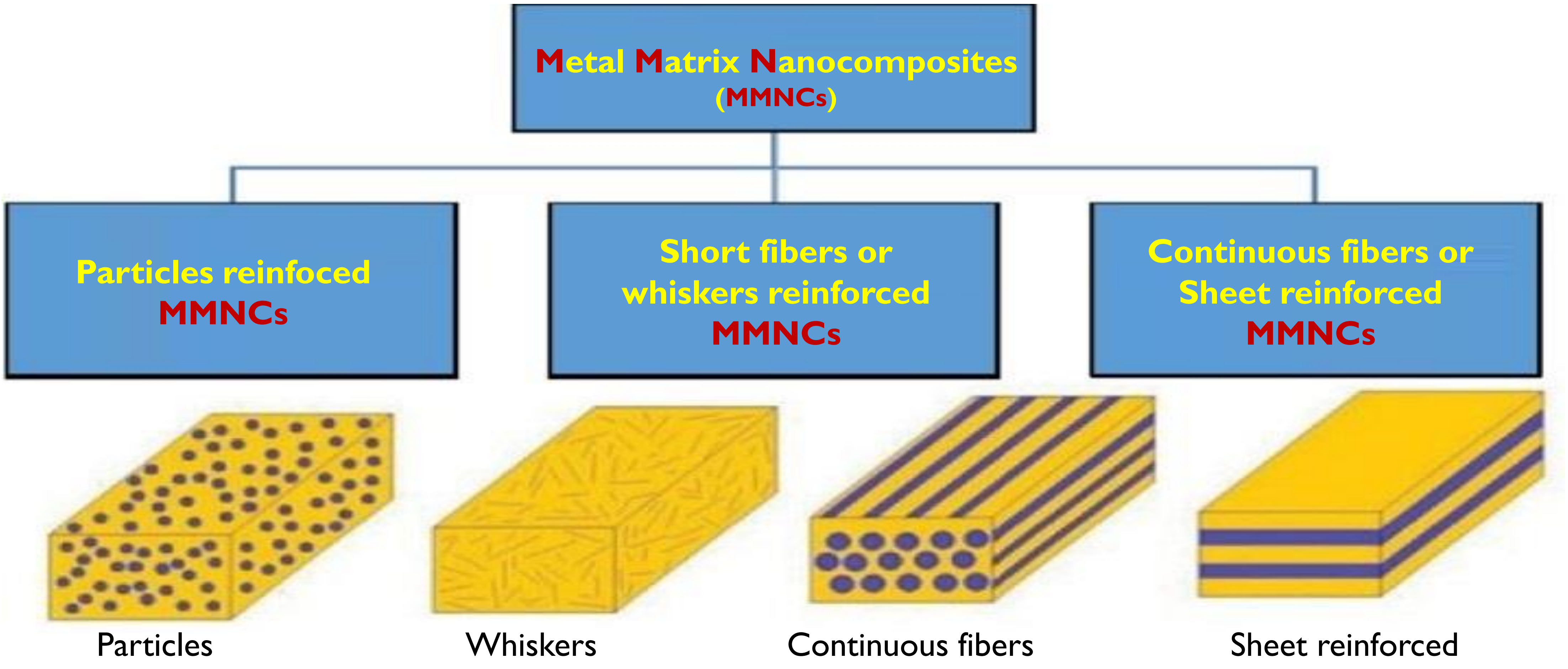
Automobile



Gas & Oil industries

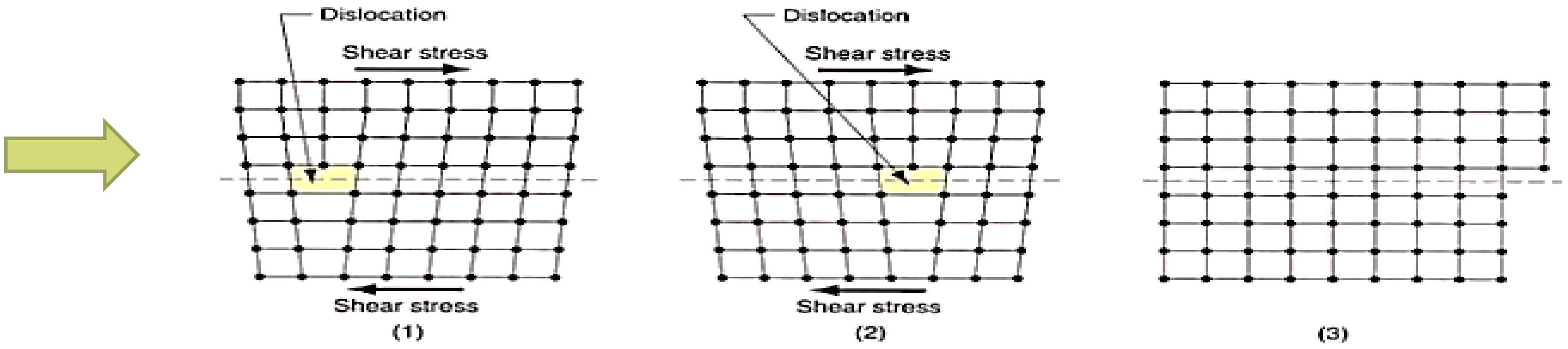
Military

Types of MMNCs



Concept of Dislocation

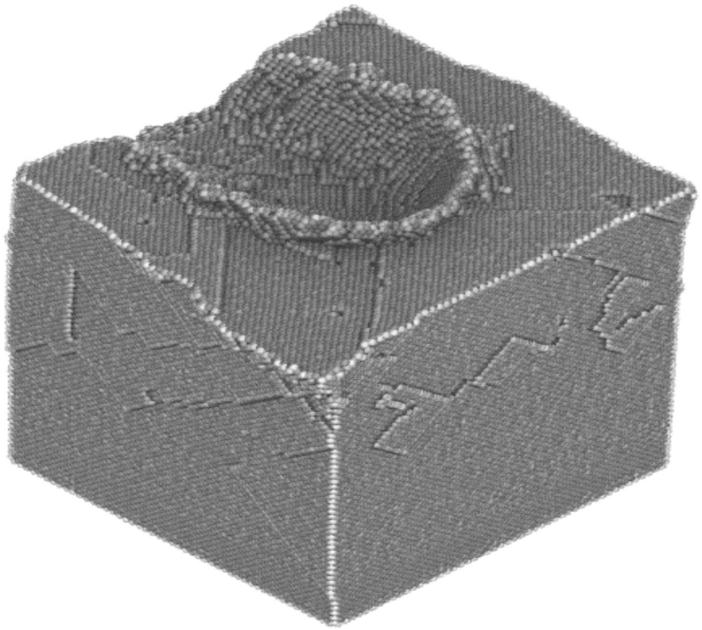
In materials science, a dislocation is a crystallographic defect or irregularity within a crystalline structure.



In the series of diagrams, movement of the dislocation allows plastic deformation to occur under a lower stress than in a perfect lattice.

Platelet or particulate nanofiller?
Which type is more effective? What are the underlying mechanisms?

The role of nanofiller geometry on the tribological behavior of aluminum-based nanocomposites



Nano Scratch Test

In miniaturized systems, surface-dependent forces like adhesion and friction can no longer be neglected because of the large surface area-to-volume ratio of structures.

So,

It is important to study tribological properties of nanodevices by different methods like scratch and indentation.

Scratching of a surface is a process where a hard tip is indented into the surface and then moved parallel to it excavating a scratch groove.

This method is well suited to test the normal as well as the lateral mechanical response of the substrate.

As the nanoscale scratching involves only the removal of a few atoms or layers of atoms, MD simulation is undoubtedly a great tool to use.

Objective of the Present work

There is a little knowledge about the effect of different nanoreinforcements on the tribological characteristics of nanodevices.

It has been demonstrated that using hard reinforcements like Silicon carbide and Graphene improves the mechanical properties of aluminum-based composites.

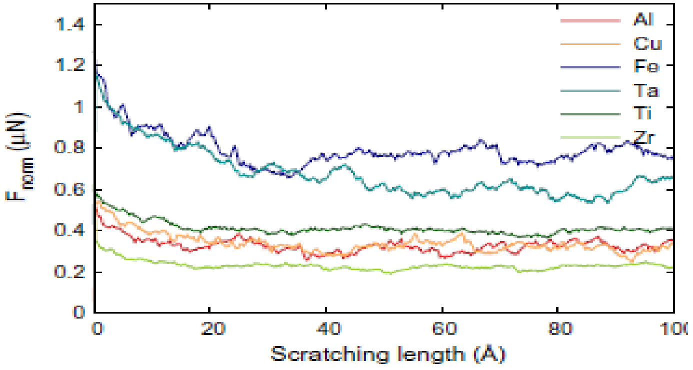
Do these reinforcements enhance the wear properties of Al matrix as well?
Which one is more effective?

To this end, Molecular Dynamics (MD) simulation was utilized to compute the friction coefficient of Al-based NCs embedded with Graphene platelets and Silicon carbide NPs.

Additionally, by analysis of the type of dislocations and their motion, the underlying mechanisms have been thoroughly investigated.

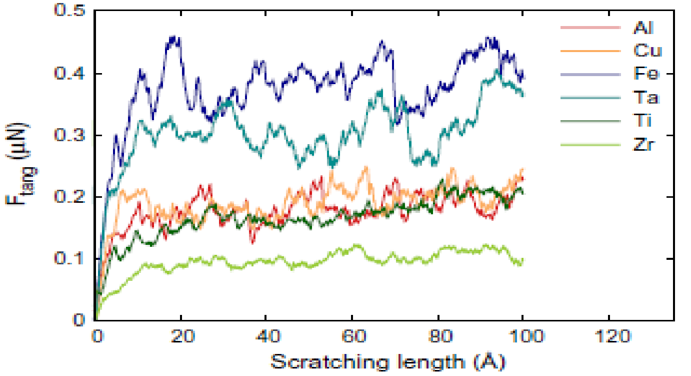
Literature Review

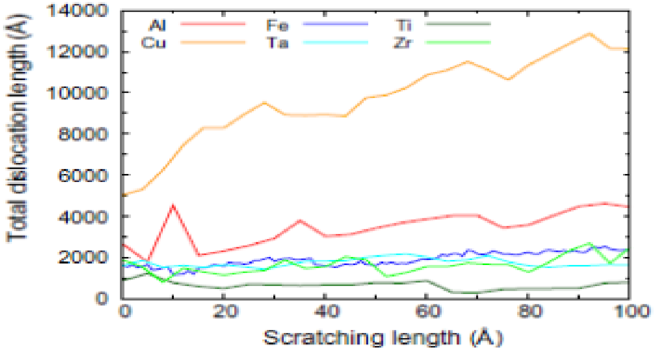
❖ Friction coefficient of different metals



Crystal	F_{norm} (μN)	F_{tang} (μN)	μ
Al	0.31	0.19	0.61
Cu	0.33	0.19	0.57
Fe	0.77	0.39	0.51
Ta	0.61	0.31	0.51
Ti	0.40	0.18	0.45
Zr	0.22	0.10	0.45

- High amount of COF for Aluminum relative to other metals





- Constant increase of the total dislocation length in FCC metals during scratch

I. A. Alhafez, C. J. Ruestes and H. M. Urbassek, *Size of the Plastic Zone Produced by Nanoscratching*, Tribology Letters, vol. 66, p. 20, 2018.

Process of Simulation

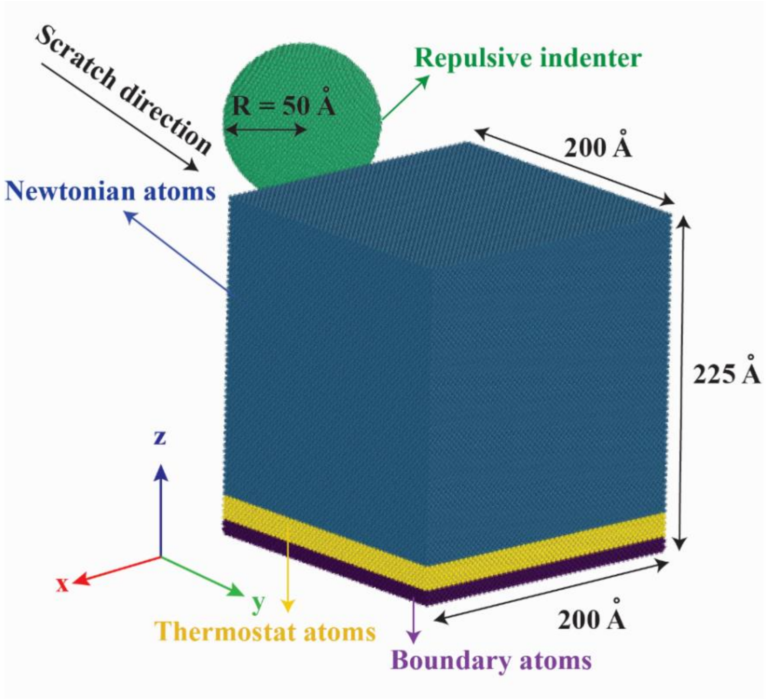
❖ All **MD** simulations were performed using the open-source **LAMMPS** code.

The basic MD cells were created in two steps:

✓ The matrix of nanocomposite consists of Al atoms were **initially** created using the built-in tools in "LAMMPS" guided by the specific metal lattice parameters.

✓ At a **later** stage, **central** holes was included to accommodate the Graphene sheet and silicon carbide nano-particles.

The size of the Aluminum samples was 20×22.5×20 nm in the x, y, & z directions respectively.



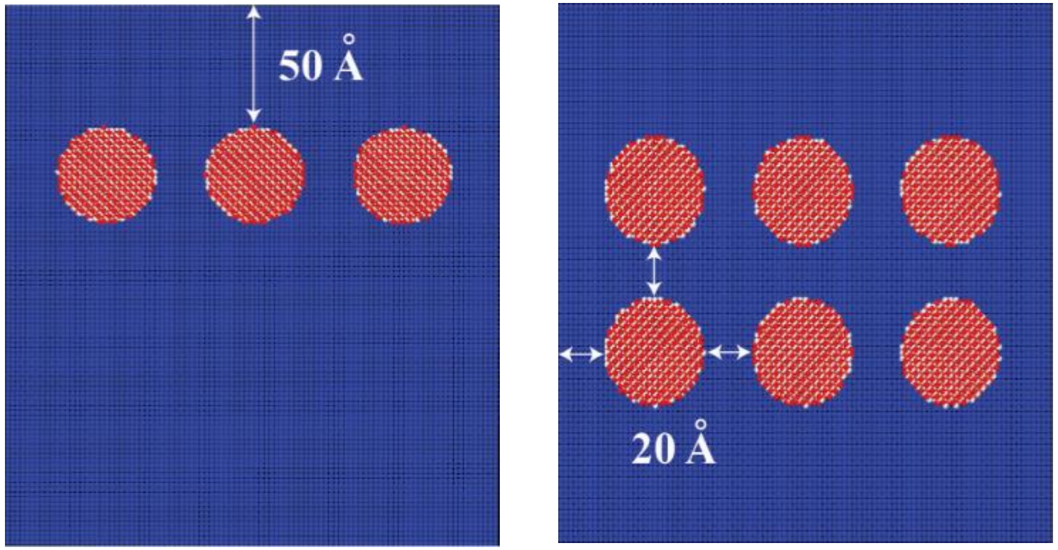
Geometrical characteristics

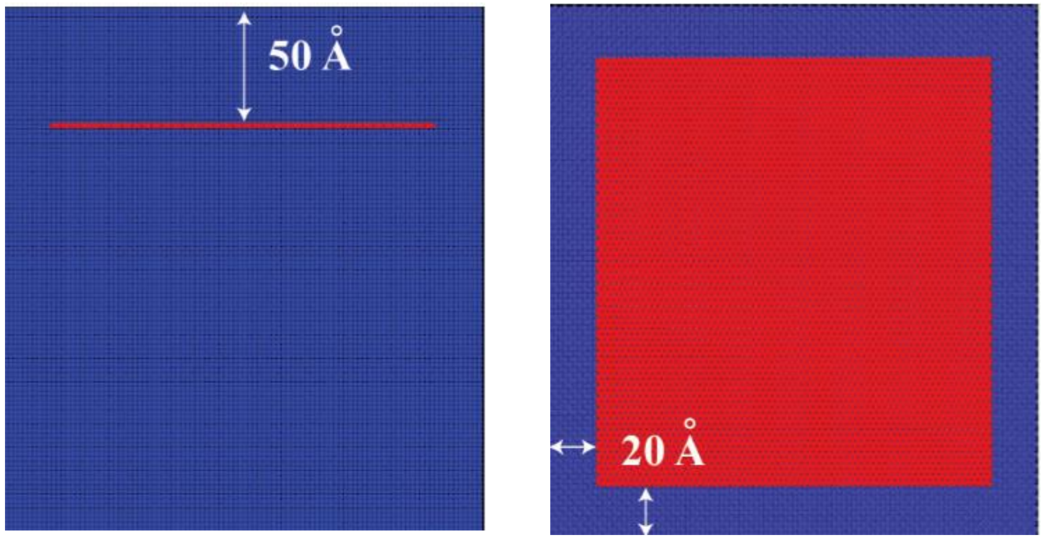
Aluminum matrix reinforced with 2.2 % VF of silicon carbide.

Si-C → Tersoff

Al-Si → Morse

Al-C → Morse





An armchair Graphene with the dimensions of 160*160 $\dot{A}$ was embedded in the Al matrix.

C-C → AIREBO

Al-C → Lennard-Jones

Process of Simulation

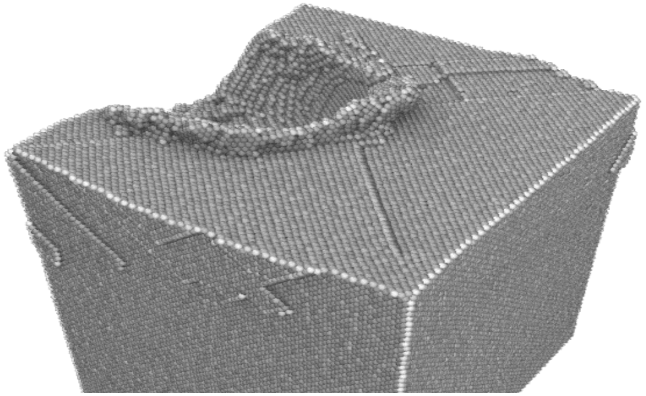
Repulsive indenter was implemented to scratch the aluminum matrix.

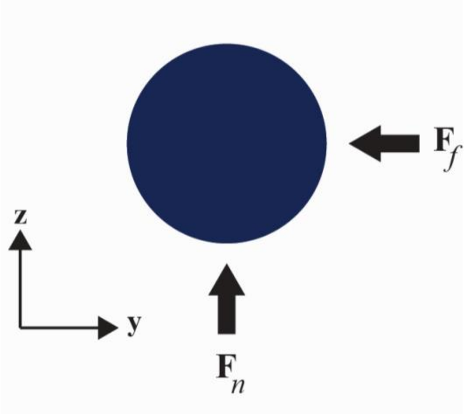
The tip has a spherical shape with a radius of R = 5 nm. It interacts in a purely repulsive way with the substrate atoms according to the following law:

$$F(r) = \begin{cases} -k(r-R)^2 & \text{if } r < R \\ 0 & \text{if } r > R \end{cases}$$

r is the distance between a substrate atom to the center of the indenter, and k = 10 $\frac{ev}{\dot{A}^3}$ is a constant.

Process of scratch





Calculated forces to estimate the friction coefficient:

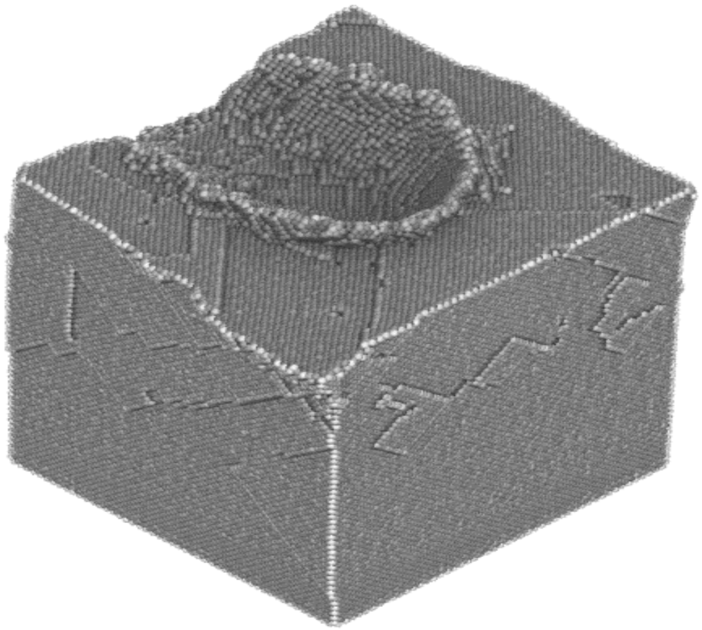
$$\mu = \frac{F_f}{F_n}$$

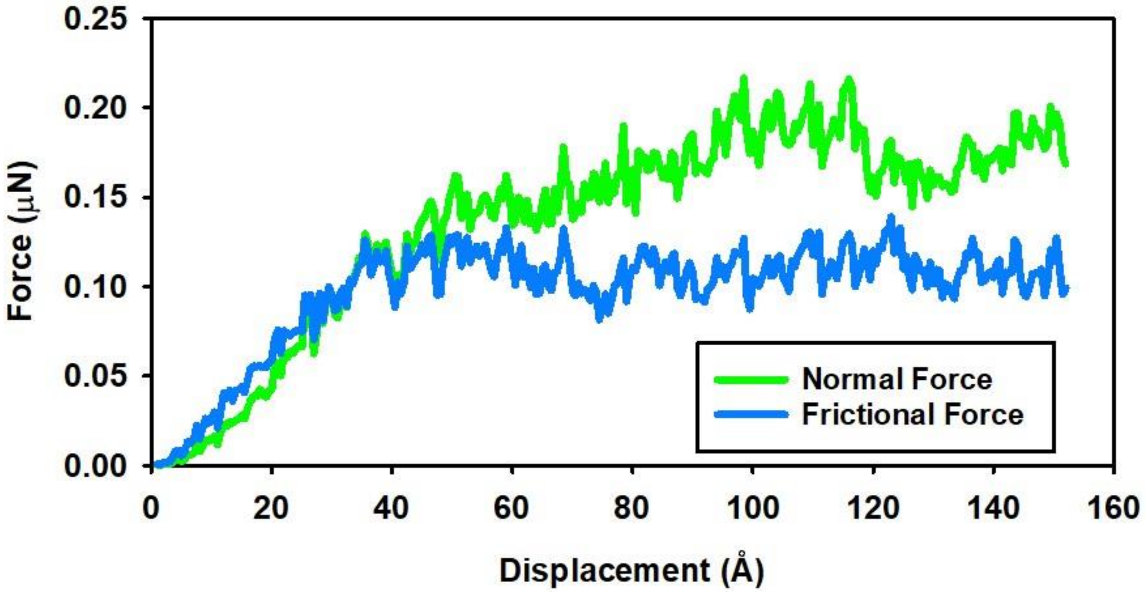
Details of MD Simulation

- ✓ The time step selected was 1 fs for all of the samples.
- ✓ Simulations were conducted in a canonical ensemble (NVT) at a constant temperature of T = 300 K.
- ✓ The tip velocity for the scratch process was chosen as 20 m/s.
- ✓ Initial velocities were sampled from a Maxwell–Boltzmann distribution at the given temperature.
- ✓ To control the temperature, the Nose´-Hoover thermostat was implemented.
- ✓ In each simulation, before applying the scratch, the MD systems were equilibrated for 40 ps.
- ✓ The box size has been chosen sufficiently large to contain the plastic zone within the system and to prevent dislocations to reach the boundaries of the simulation box.

Validation of the Model

Pure Aluminum under scratch:





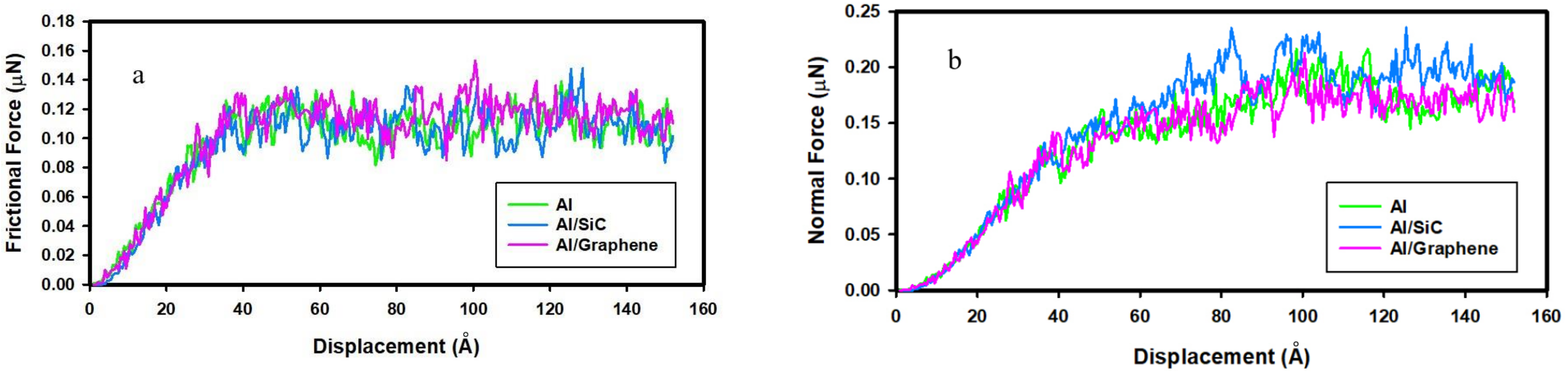
Force-Displacement curve of the sample

These results are in good agreement with the data published by Urbassek et al. They reported 0.61 for the friction coefficient of pure Al.

sample	F_x (μN)	F_y (μN)	μ
Aluminum	0.110	0.179	0.61

I. A. Alhafez, C. J. Ruestes and H. M. Urbassek, *Size of the Plastic Zone Produced by Nanoscratching*, Tribology Letters, vol. 66, p. 20, 2018.

Scratch forces and COF for different samples

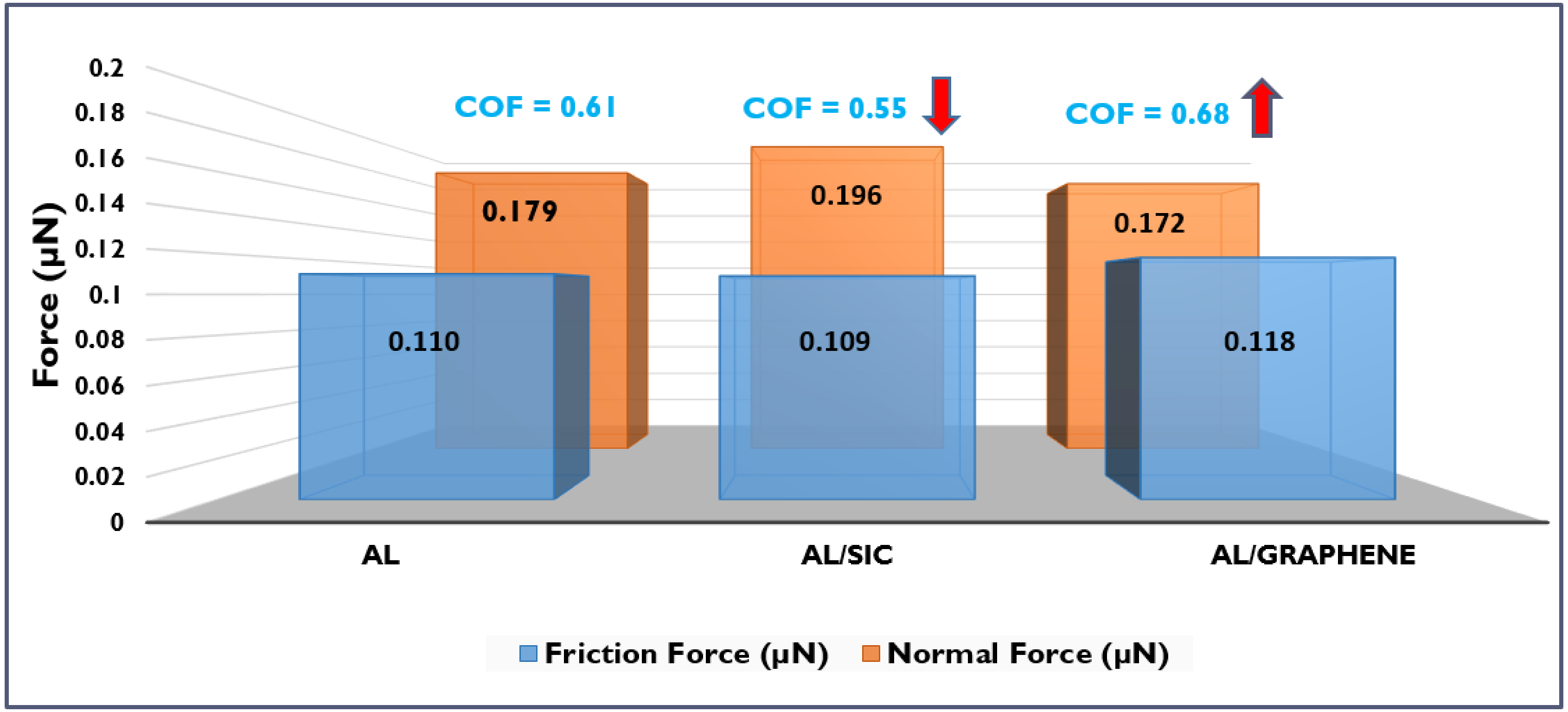


Force-Displacement curves of the samples

Friction coefficient for the introduced samples

Sample	Al	Al/SiC	Al/Graphene
COF	0.61	0.55	0.68

Scratch forces for the different samples



Average of frictional and normal forces during scratch

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Al/Graphene

$\frac{F_x}{F_y}$

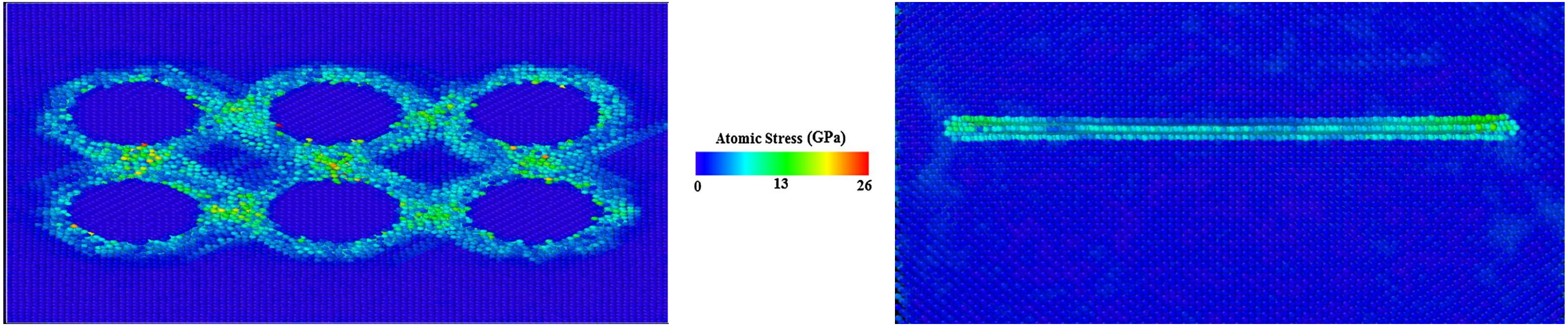
μ

Al/SiC

$\frac{F_x}{F_y}$

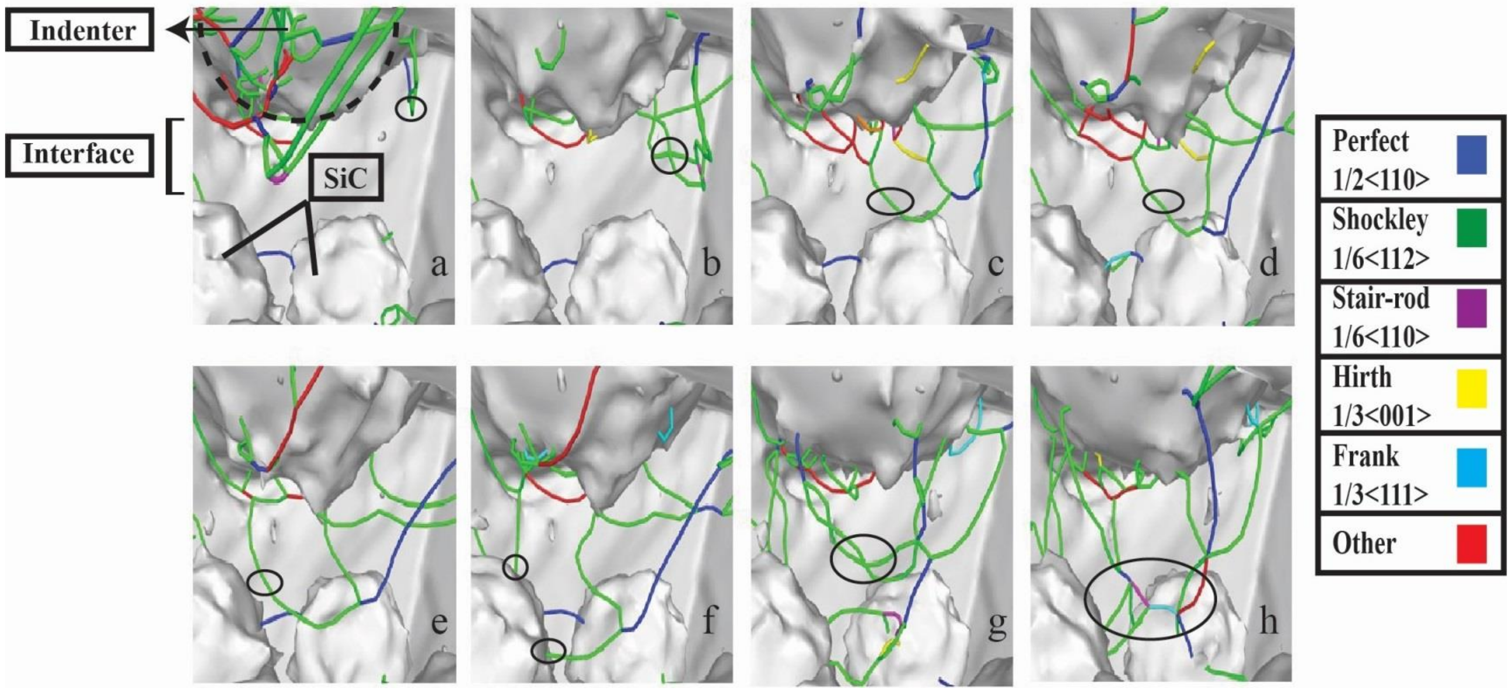
μ

Interface: Different behavior due to stress concentration



Stress concentration in SiC/Al interface motivates the dislocation nucleation & complex interactions between them.

Dislocations and SiC NPs:
DXA-based proposed mechanism



SiC acts as an obstacle for dislocations movement → Dislocations accumulate near the interface of SiC particles forming a special zone as a dislocation source producing a large number of new dislocations under indenter.

← This phenomenon causes this area to be strengthened, which is called as Orowan strengthening.

← $\frac{F_x}{F_y}$ ↑

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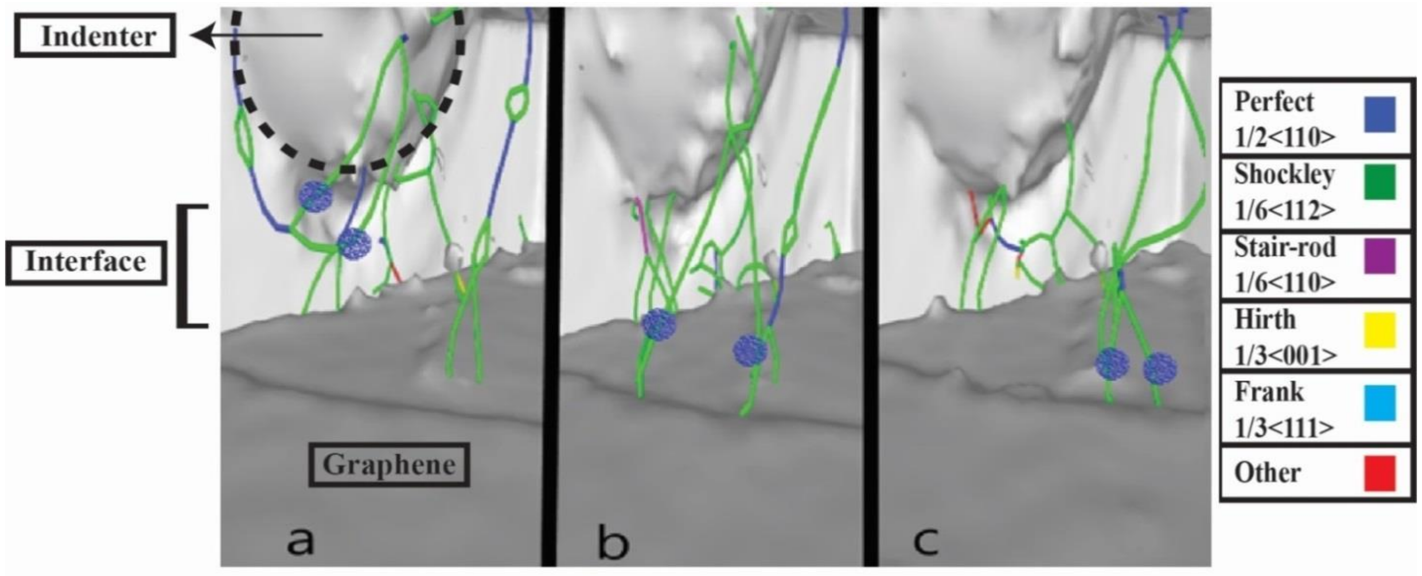
Dislocations and **Graphene** platelet:
Towards the governing **mechanism**



Smooth movement of dislocations on the graphene interface → Increase in the dislocation density ahead of indenter tip → More plastic deformation in front of the indenter

$\frac{F_x}{F_y}$ ↑

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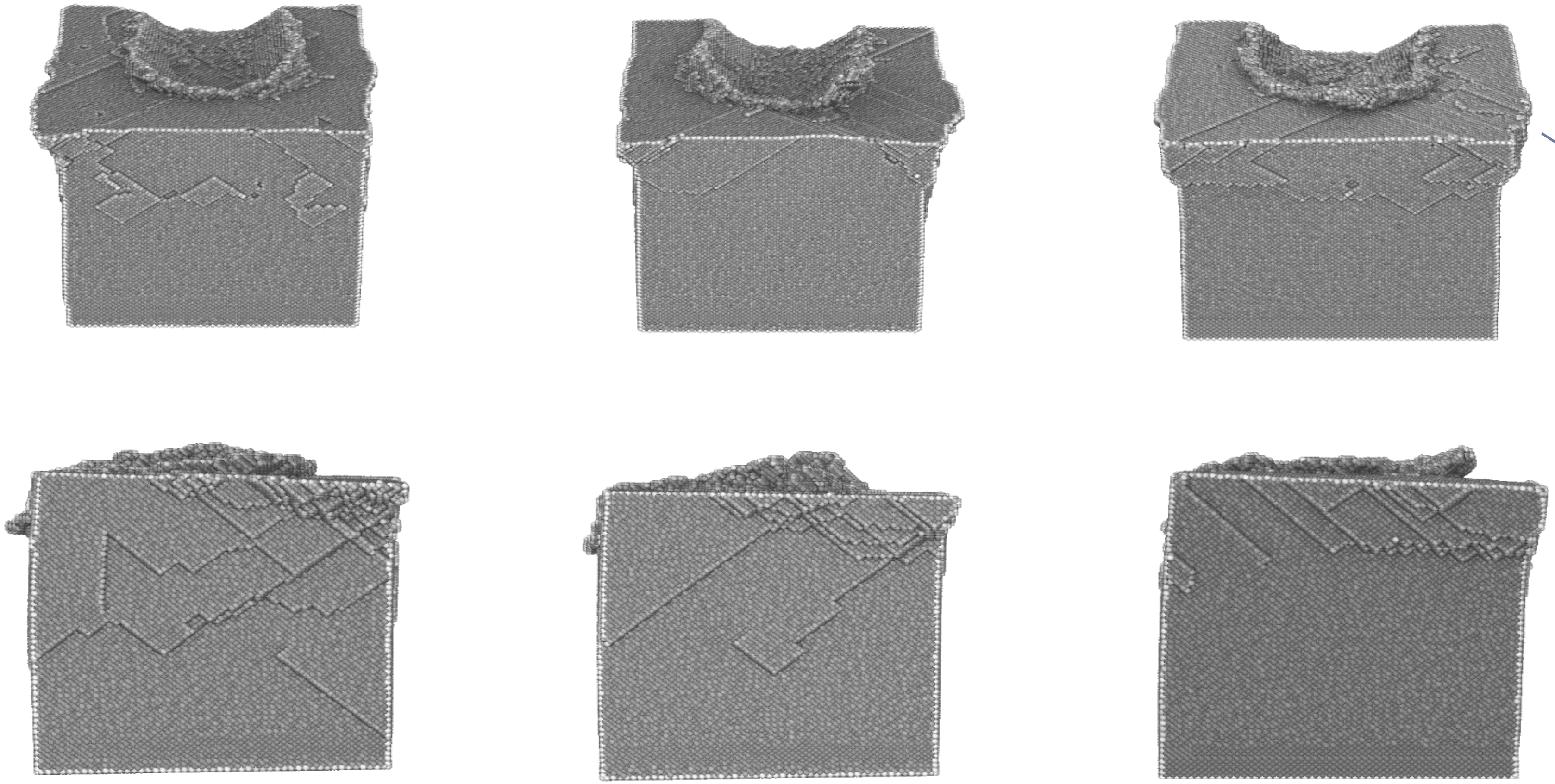
Samples after scratch



Al/SiC Al Al/Graphene

More plastic deformation was observed on the lateral and front faces of Al/Graphene sample caused by dislocations movement and adsorption to surface.

Summary & Concluding Remarks

❖ In the present work, MD was employed to compute the friction coefficient of Aluminum nanocomposites embedded with SiC and Graphene during scratching test.

❖ It was shown that SiC NPs reduce friction coefficient, while Graphene platelets increase it relative to the pure aluminium.

❖The dislocation-based mechanisms were also thoroughly studied.

❖ The tribological behavior of MMNCSs is highly dependent on the geometrical characteristics of the nanofillers.

Thanks for Your Attention