RWTH AACHEN UNIVERSITY

# Effect of Graphene coating on Hypervelocity Impact Resistance of Aluminium: A Molecular Dynamics approach

Final Project Report: Molecular Dynamics and Multiscale Modeling of Materials

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## 1. Introduction:

Hypervelocity is very high velocity, approximately over 3,000 meters per second. This is especially relevant in the field of space exploration and military in anything from minor component degradation to the complete destruction of a spacecraft or missile. Graphene, an allotrope of carbon has a special set of properties which sets it apart from the other allotropes. In relation to its thickness, it is about 100 times stronger than the strongest steel. Yet its density is dramatically lower than any steel. Hypervelocity impact simulations were conducted on Aluminium, one of the most popular and lightweight metals, to study its resistance to these impacts. The resistance to the impacts was measured in terms of the reduction in kinetic energy of the indenter, upon impact with the block. The block was further coated with graphene, and the reduction in energy was monitored.

## 2. System Construction:

System Modeling and simulations were performed using LAMMPS and OVITO was used for post processing of the data.
An aluminium block of volume 135 x 135 x 135 (nm^3) was used for the simulations. Further, it was coated with one, two and three layers of graphene sheets respectively, all with an area of 135 x 135 (nm^2). A rigid diamond indenter of diameter 50 nm was used for simulating a Hypervelocity impact.

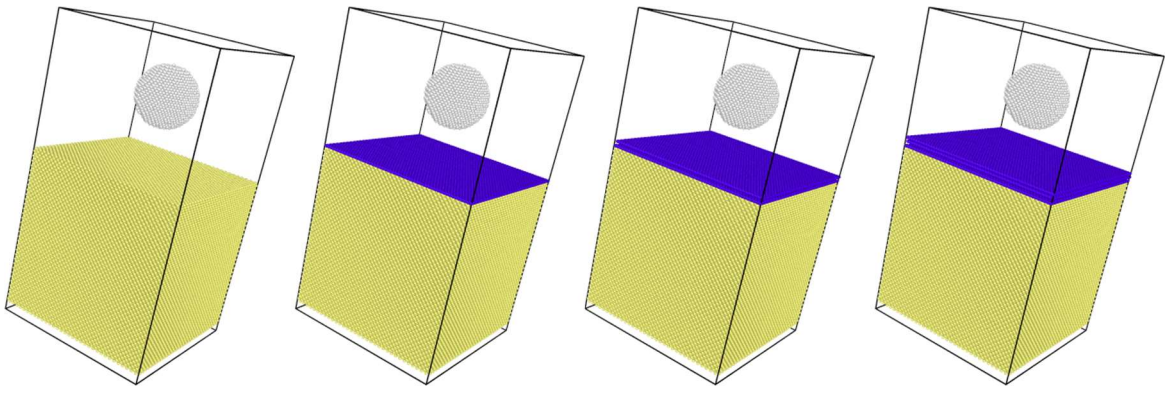

**Figure 1. (a)** Aluminium Block without graphene sheets. **(b)** Aluminium Block with 1 graphene sheet. **(c)** Aluminium Block with 2 graphene sheets. **(d)** Aluminium Block with 3 graphene sheets.

**3. Simulation Setup:**

Periodic boundary conditions were defined in the x and z direction, with non-periodic boundary condition in the y direction.

The system consisted of three groups of atoms:

- Group 1: Graphene (Carbon).
- Group 2: Diamond Indenter (Carbon).
- Group 3: Aluminium Block (Aluminium).

The following atomic interactions were defined:

- C-C (Graphene): The adaptive intermolecular reactive bond order (AIREBO) potential was used to consider both the short- and long-range interactions between the atoms.
- Al-Al (Aluminium Block): EAM potential.
- C-Al (Graphene – Aluminium Block): Morse potential.
- C-Al (Diamond indenter – Aluminium Block): Morse potential.
- C-C (Graphene – Diamond Indenter): Lennard Jones potential.
- C-C (Diamond Indenter): None. Since it was considered as a rigid body.

For minimization, the Conjugate Gradient (CG) method was used. Equilibration of the system was carried out using the NVE (constant volume, constant energy) ensemble. Since, the NVE ensemble does not control the temperature, velocity scaling was used to maintain a system temperature of 300K.

The aluminium block was divided into three different zones: fixed atoms zone, heat sink atoms zone and Newtonian atoms zone. The fixed atoms were kept fixed to provide a support to the block for the impact. The heatsink atoms were used to absorb the excessive heat after the impacts. The motion of the Newtonian atoms was determined by the forces produced by Newton's equation of motion.

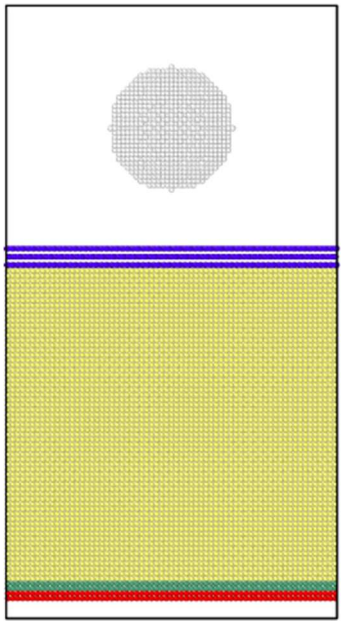

**Figure 2.** Fixed atoms (red). Heatsink atoms (green). Newtonian atoms (yellow).

After the system was equilibrated, impact simulations were carried out at different velocities with different layers of graphene coating on the aluminium block. The diamond indenter was specified as rigid during the impact simulations as the deformation of the indenter was not in the scope of the project.

**4. Results and discussions:**

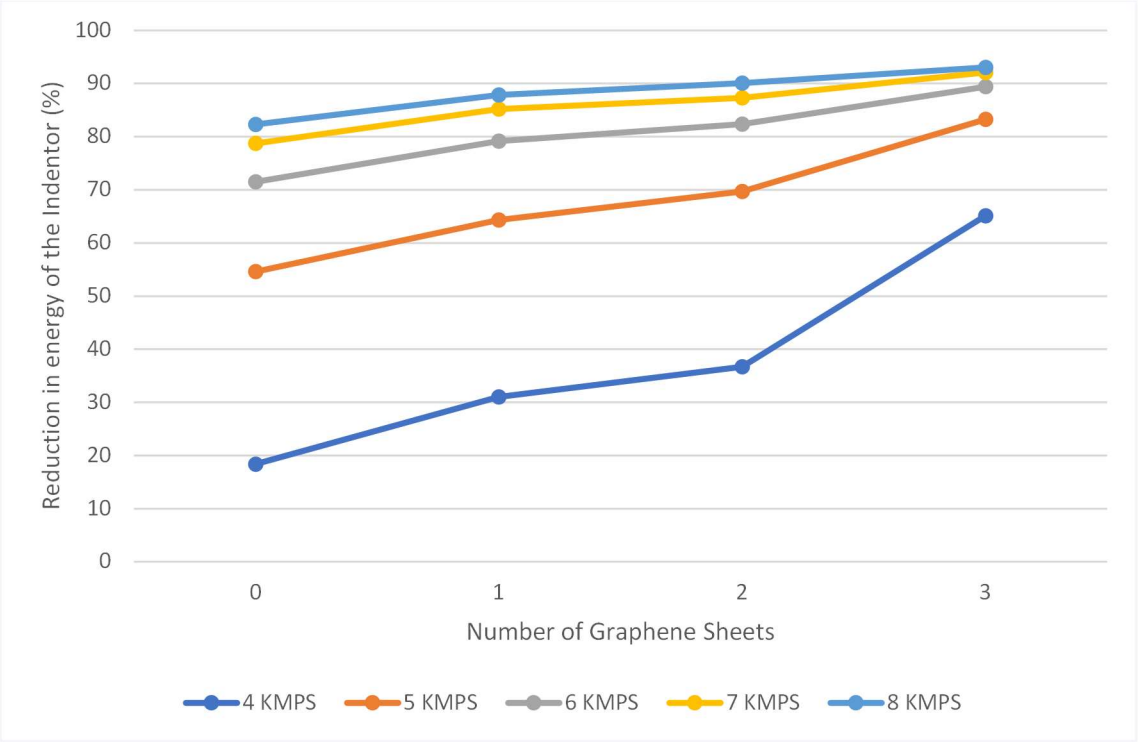


**Figure 3.** Reduction in energy of the Indenter (%) vs Number of Graphene sheets for different impact velocities.

The reduction in the kinetic energy of the indenter was monitored after 1 picosecond of the impact.

Figure 3 predicts a trend between the reduction in energy of the indenter upon impact vs the number of graphene sheets coated on the block, for different impact velocities. It can be clearly observed that as the number of graphene sheets are increased, the reduction in energy of the indenter increases, basically it slows down faster.

It can also be observed that as the impact velocity increases, the difference in reduction in energy, with increase in graphene sheets decreases. This can be attributed to the fact that the graphene sheets start to fracture as the velocity increases and their ability to absorb the energy reduces.

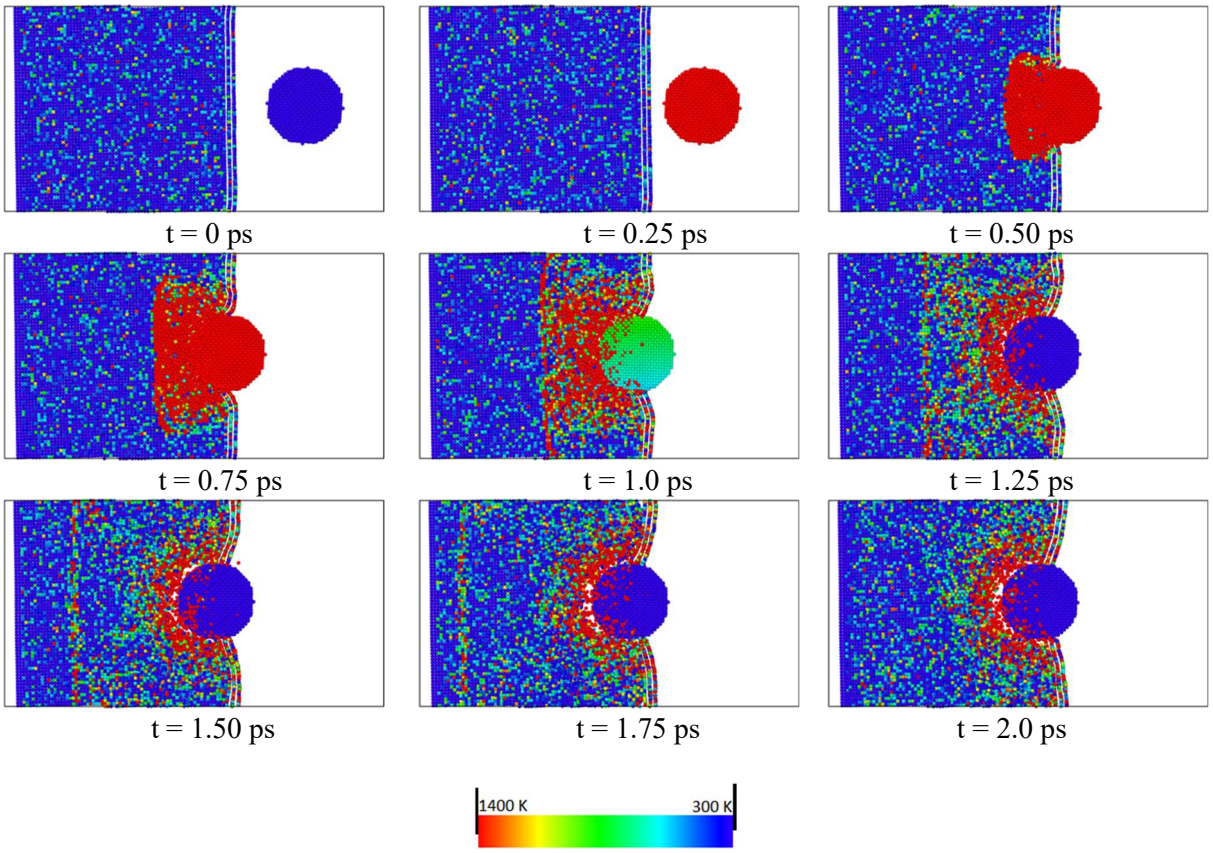


**Figure 4.** Temperature distribution at different timesteps for impact velocity of 8KMPS with 3 graphene sheets. A slice of 10 angstrom has been used to view the geometry.

From figure 4, the temperature distribution of the system can be observed. It can be clearly seen that the temperature near the heat sink atoms is the lowest and is higher near the impact area.

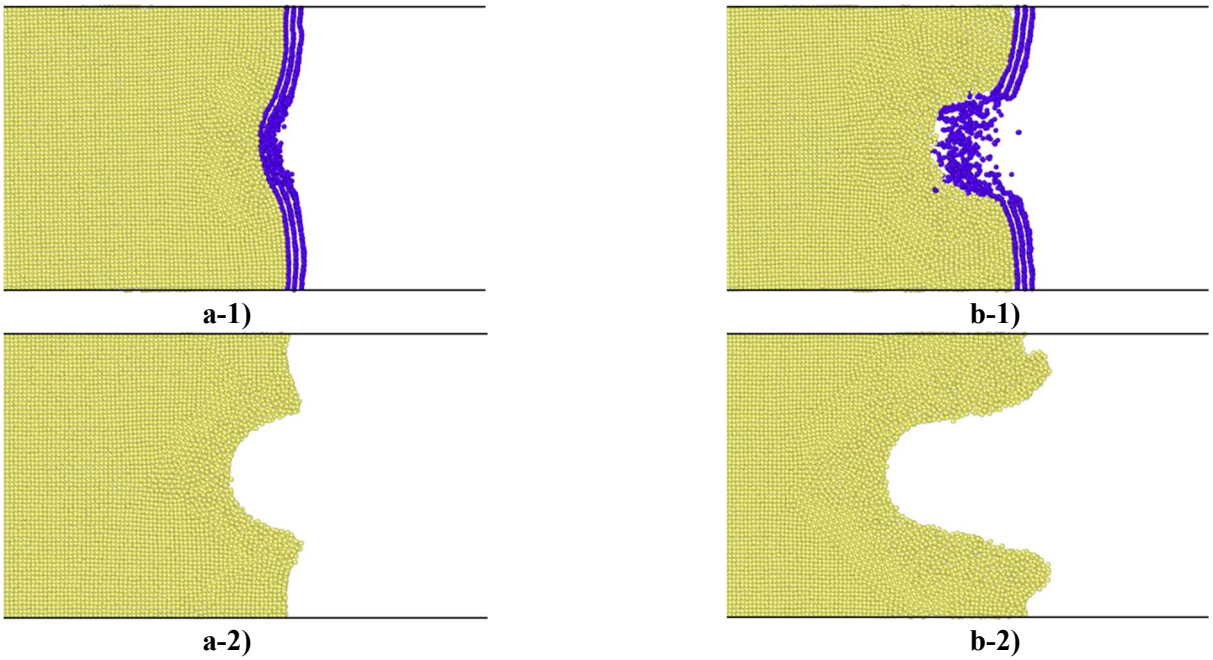

**Figure 5. a-1)** Penetration depth with 3 graphene sheets at 4KMPS. **a-2)** Penetration depth without graphene sheets at 4KMPS. **b-1)** Penetration depth with 3 graphene sheets at 8KMPS. **b-2)** Penetration depth without graphene sheets at 8KMPS. A slice of 10 angstrom has been used to view the geometry.

From figure 5 it can be observed that the penetration depth reduces with addition of 3 graphene sheets. The penetration depth can also be related to the damage caused to the block. Thus, the penetration depth must be as less as possible. The results are in conformance with the desired physical behaviour.

**5. Conclusion:**

The results obtained in the project clearly imply that coating a metal with graphene can improve its resistance to Hypervelocity impacts. The above study can be extended to other metals to establish confidence in the observed trends.

**References:**

1. https://lammps.sandia.gov/doc/Manual.html
2. https://lammps.sandia.gov/mail.html
3. https://en.wikipedia.org/wiki/Hypervelocity
4. https://en.wikipedia.org/wiki/Graphene
5. https://www.researchgate.net/publication/324477174_A_novel_nonlinear_nano-scale_wear_law_for_metallic_brake_pads
6. https://www.researchgate.net/publication/332217214_Nanoindentation_of_Graphene-Reinforced_Silica_Aerogel_A_Molecular_Dynamics_Study

```
# Equilibration script

# Atom Definition

units metal
dimension 3
boundary p f p
atom_style full # to consider molecular effects into account

# Simulation box and geometry modeling

read_data geoinput.data # read geometry data file

group graphene type 1 # specify atom number
group projectile type 2
group alblock type 3

region fixedatoms block INF INF 64 68 INF INF units box # select atoms to create fixedatoms for support
group fixedatoms region fixedatoms

region thermoatoms block INF INF 59 63 INF INF units box # select atoms to create heat sink
group thermoatoms region thermoatoms

# ForceFields

pair_style hybrid airebo 3.0 eam/alloy morse 2.5 lj/cut 2.5
pair_coeff * * airebo CH.airebo C NULL NULL
pair_coeff * * eam/alloy Al99.eam.alloy NULL NULL Al
pair_coeff 1*2 3 morse 0.4691 1.738 2.246
pair_coeff 1 2 lj/cut 1 1 2.5
pair_coeff 2 2 none # since projectile is rigid

# Minimization

min_style cg
minimize 1.0e-10 1.0e-10 1000 10000

# Equilibration

velocity all create 300 1234567 mom yes rot yes sum no dist gaussian
reset_timestep 0
timestep 0.0005 # smaller timestep for better accuracy

fix 1 all nve
fix 2 all momentum 1 linear 1 1 1
fix 3 projectile move linear 0 0 0
fix 4 all temp/rescale 25 300.0 300 0.02 0.5 # to maintain a temp of 300K
fix 5 projectile rigid single
fix 6 fixedatoms move linear 0 0 0

thermo 100
thermo_style custom step lx ly lz press pxx pyy pzz pe temp

run 50000

unfix 1
unfix 2
unfix 3
unfix 4
unfix 5
unfix 6


write_restart restart_equilibratedg_system.equil # input file for impact simuations

write_data equilibrated.data # to view equilibrated system
```

```
# Impact Simulation script

read_restart restart_equilibratedg_system.equil #read equilibrated system

#------------------Force Fields--------------

pair_style hybrid airebo 3.0 eam/alloy morse 2.5 lj/cut 2.5
pair_coeff * * airebo CH.airebo C NULL NULL
pair_coeff * * eam/alloy Al99.eam.alloy NULL NULL Al
pair_coeff 1*2 3 morse 0.4691 1.738 2.246
pair_coeff 1 2 lj/cut 1 1 2.5
pair_coeff 2 2 none


compute keproj projectile ke #compute kinetic energy of projectile
compute keatom all ke/atom
compute peatom all pe/atom
variable kb equal 8.671333262145e-5
variable alltemp atom (2*c_keatom)/(3*v_kb) #compute temperature of atoms

reset_timestep 0
timestep 0.0005 # smaller timestep due to high velocities

thermo 100
thermo_style custom step cpu temp pe vol etotal ke c_keproj
dump RESULTS all custom 100 RESULTS_*.cfg id type x y z vx vy vz fx fy fz c_keatom
v_alltemp v_blocktemp
thermo_modify lost ignore flush yes
run 200

velocity projectile set 0.0 80.0 0.0 units box # specify linear velocity

fix 1 all nve
fix 2 all momentum 1 angular
fix 3 projectile rigid/nve single # specify projectile as rigid
fix 4 fixedatoms move linear 0 0 0 # fix atoms for support
fix 5 thermoatoms temp/rescale 25 300.0 300 0.02 0.5 # maintain a temperature of
300K to create a heat sink

run 5000
```