Supplementary Information

A novel nonlinear nano-scale wear law for metallic brake pads

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Average temperature of Newtonian atoms of the Fe brake pad as a function of normalised simulation time for different velocity loadings

Figure S1 shows the temperature-time history plot of the Fe brake pad in case of different velocity loadings. The three phases are clearly identified in the figure. First (phase I), up to a normalised simulation time of 50 time unit, the constant average temperature of 300 K was maintained. The high average temperature was observed (except \( v < 0.1 \) nm/ps) from the normalised simulation time of 50 to 80 time unit (phase II), and the average temperature of the Newtonian atoms of the brake pad was decreased significantly from normalised simulation time of 80 to 100 time unit (phase III). For high velocity loadings (\( v \gtrsim 0.1 \) nm/ps), due to the sudden and high impact between the bottom layer of Newtonian atoms and the rigid disc, the contact atoms acquire extreme velocities, and ultimately extreme fluctuations in temperatures were observed.
Figure S1. Average temperature of Newtonian atoms of the Fe brake pad as a function of normalised simulation time for different velocity loadings.
Average temperature of Newtonian atoms of Al, Cu and Fe of Model III versus applied constant angular speed $\omega$ of diamond disc

As observed, in the case of Model II (illustrated in the manuscript Figure 4), for Model III, the average temperature of Al, Fe and Cu also increases with increasing angular speed of the disc. The average temperature of all the considered metallic brake pads shows a power law dependence on the angular speed of the disc.

Figure S2. Average temperature of Newtonian atoms of Al, Cu and Fe of Model III versus applied constant angular speed $\omega$ of diamond disc. Power law fits to the simulation data are shown with dotted lines.
Average temperature of different regions of Fe brake pad Newtonian atoms versus simulation time

Figure S3, shows the average temperature variation with respect to the simulation time. In order to study the average temperature variations, Fe brake pad Newtonian atoms can be divided into top half and bottom half. Up to a simulation time of 100 ps, constant average temperature of 300 K was maintained in all the regions. As the bottom half Newtonian atoms come first and remain in contact with the disc, its temperature rises to \(~1000\) K after 100 ps, however, the top half experience the temperature of \(~650\) K.

![Figure S3. Average temperature of different regions of Fe brake pad Newtonian atoms versus simulation time.](image-url)
Average Temperature of the Fe brake pad Newtonian atoms of Model I, II and III versus applied constant angular speed $\omega$ of diamond disc

Figure S4, shows the plot of average temperature of all the three materials, Al, Fe and Cu versus angular velocity. As rotating angular speed of the disc increases, there was increase in the average temperature of the Fe brake pad Newtonian atoms. The average temperature shows a power law dependence on the angular speed of the disc. As already discussed, Model II and III, show the power law relationship with an exponent of 0.38, whereas Model I with an exponent of 0.26. Hence, with respect to feasibility and also computational cost, Model II was a preferred choice for further studies.

![Graph showing average temperature vs angular speed for Model I, II, and III](image)

**Figure S4.** Average Temperature of the Fe brake pad Newtonian atoms of Model I, II and III versus applied constant angular speed $\omega$ of diamond disc.
Normal reaction force

In Figure S5, the normal reaction force was plotted against simulation time for the Cu brake pad with $\omega = 12.56$ rad/ns and $v = 0.01$ nm/ps. In the second phase of loading, the normalised force was nearly constant between $\sim 80$ and $\sim 140$ ps simulation time. Therefore, this constant force was considered for that particular velocity loading, and further calculations were carried out using this force value.

Figure S5. Normal reaction force variation with simulation time for the Cu brake pad with $\omega = 12.56$ rad/ns and $v = 0.01$ nm/ps.
Calculation of the total number of atoms lost from the Fe break pad using the material loss and the geometry based method

As shown in the Figure S6, the total number of atoms lost from the Fe material brake pad is calculated using the material loss and the geometry based method. The calculated number of atoms lost was found to be in good agreement.

Figure S6. Calculation of the total number of atoms lost from the Fe break pad using the material loss and the geometry based method.