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Research Letter

An Analytical Description of the Frictional Behaviour of a Titanium Alloy

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In recent years, significant effort has been put in the enhancement of our understanding of the physics and mechanics of moving objects under contact. Developed theoretical models can not fully account for the observed frictional behaviour of materials due to the lack of understanding of the interaction processes which occur at the microscopic level. In this paper, an analytical contact model will be described and its application to a titanium alloy will be presented. Conclusions will be drawn on the ability of this model to describe different friction regimes. The inclusion of additional factors which impact on frictional behaviour will be discussed, as well as the derivation of constitutive equations and their utilisation in continuum models.

1. INTRODUCTION

The movement of an object along a surface in the macro- or microscales is resisted by forces commonly referred to as friction. The basic laws of macroscopic friction developed by Amontons [1], although not holding in every condition of stress, temperature, velocity, and length scale, have far outlived a number of theoretical attempts to provide a clear explanation of friction as well as a unified theory for friction in both the macroscopic and the microscopic levels. The difficulty in identifying the origin and method of development of friction at microscopic level lies with the enormous number of contacts which develop over time and are difficult to characterise. A number of approaches have been proposed over the past decades in order to explain how friction develops at the microscale and how it influences the macroscopic behaviour of materials (e.g., [2–4]).

2. ANALYTICAL CONTACT MODEL

In the present study, a contact model, originally developed by Persson [5] and later taken up by Filippov et al. [6], has been utilised in order to model the sliding motion of two plates by relating microscopic phenomena to the macroscopic motion of a top plate relative to a stationary bottom plate. The model has been modified in order to reflect the change in microscopic friction due to the release of energy during the rupture of molecular bonds. Further, a simplification in the case of strong bonds has been applied. The effectiveness of this model will be demonstrated during the presentation of the results.

In the model, two rigid surfaces are connected by junctions that spontaneously break and form upon contact. The junctions are assumed to behave as elastic springs with a force constant κ and a rest length $l^{(0)}$. A spring of constant K is exerting the necessary force to move the top surface at a constant velocity V. The equation of motion of the driven surface follows a Maxwell-type equation:

$$M\ddot{X} + \eta\dot{X} + F_b + K(X - Vt) = 0, \tag{1}$$

where the force due to the interaction between the junctions and the driven surface is F_b, and η is the damping coefficient. Coefficients K and η are material properties, closely related to the material elastic constants. The force F_b is given by the equation

$$F_b = \sum_{i=1}^{N} q_i f_i^{(x)}, \tag{2}$$

where q_i indicates the state of the junction (1 for formed junction, 0 for breached junction).

The elastic force f_i from the junction formed is given by Hooke's law, with l_i being the length of the junction and $l^{(0)}$ the distance between the plates:

$$f_i = \kappa\left[l_i - l^{(0)}\right]. \tag{3}$$

The projection of this force in the direction of motion is $f_i^{(x)} = f_i x_i / l_i$, x_i being the bond extension in the X-direction ($[x_i + l^{(0)}]^{1/2} = l_i$). The top surface is continuously forming junctions that hinder sliding and extend, as well as breaking junctions with the bottom stationary surface.

Each model junction extends and contracts as the two surfaces slide on each other, which may be represented by

$$\dot{x}_i = q_i \dot{X} + \lambda \delta x_i, \tag{4}$$

where δ is 1 directly after the bond rupture and 0 at all other instances. The relaxation constant λ characterises the approach of a junction to its equilibrium length, an action different for each junction, which leads to the elastic forces being different for each individual junction.

The state q_i of the individual junction can be described in time through equation

$$\begin{aligned} q_i(t + \Delta t) = {} & q_i(t) - q_i(t)\theta(\xi_i - \Delta t k_{\text{off}}) \\ & + [1 - q_i(t)]\theta(\xi_i - \Delta t k_{\text{on}}), \end{aligned} \tag{5}$$

where Δt is the time step, ξ_i is a random variable in the interval (0,1) (obtained through a Park-Miller random number generator [7]) and $\theta(z)$) is the Heaviside step function for the description of the stochastic fracture (creation) of a junction that occurs for $\xi_i > \Delta t k_{\text{off(on)}}$. The rate of creation and fracture of junctions is k_{on} and k_{off}, respectively.

Junctions can be of two types: weak or strong junctions, where the junction energy is slightly larger or much larger than $k_B T$, respectively (k_B is the Boltzmann constant). The time-dependent fracture rate then is

$$k_{\text{off}}(l_i) = \begin{cases} k_0 \exp(\beta f_i \Delta x), & \text{weak junction} \\ k_0, & \text{strong junction } (f_i/f_c \longrightarrow 0), \end{cases} \tag{6}$$

where k_0 is the spontaneous rate of junction fracture when there is no external force present, $\beta = 1/k_B T$, Δx is the difference between the maximum and minimum of the junction reaction potential, and f_c is the critical force at which the potential barrier disappears and bond dissociation occurs in the absence of thermal fluctuations.

The junction creation is characterised by the rate k_{on}, which for simplicity is assumed to depend only on the age of the contact τ (i.e., the time that the free end of the junction is exposed to the moving interface):

$$k_{\text{on}} = k_{\text{on}}^0 g(\tau, \tau_0), \tag{7}$$

with k_{on}^0 being the rate of junction creation for a stationary contact, τ_0 some critical junction age, and g a modified stepwise function ($g = 0$ for junction age $\tau \ll \tau_0$, $g = 1$ for $\tau > \tau_0$ and $g = \sin(\tau/\tau_0 \cdot \pi/2)$ for $0 < \tau < \tau_0$). Contact time τ is related to sliding velocity and the typical length scale of the contact α through the equation $\tau = \alpha/\square$. The characteristic time-scale τ_0 necessary for junction creation is used to define a critical velocity $V_0 = \alpha/\tau_0$. Above this, velocity junctions cannot be formed. This is necessary in order to accurately represent stick-slip conditions.

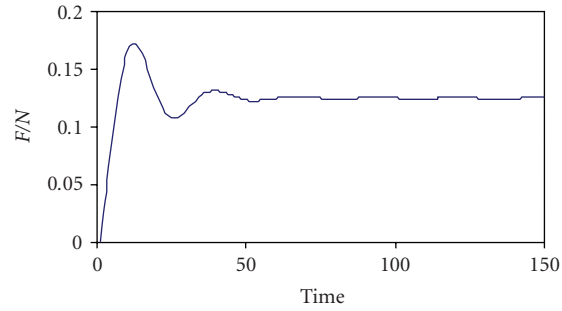

Figure 1: Temporal variation of friction force, as calculated by the model for parameter values $V = 0.5$, $N = 300$, $K = 150.0$, $\eta = 75.0$, $\kappa = \lambda = 0.1$, $l^{(0)} = \alpha = \Delta x = 1.0$, $k_0 = k_{\text{on}}^0 = 0.1$, $\tau_0 = 2.0$, $\Delta t = 1.0$.

3. RESULTS AND DISCUSSION

The model was initially applied to study the frictional behaviour of a titanium alloy under constant sliding velocity and temperature, for which experimental data were available [8]. A large number of junctions ($N = 300$) were assumed, representative of the specimen size in the experiments (of the order of millimetres), and the friction force per junction was calculated through the combination of microscopic and macroscopic friction forces; $N = 300$ was deemed to be a suitably large number of junctions at the micron scale, in order to obtain with the available computing resources a statistically correct result for the averaged frictional force. Since this present work concerns the study of the *behaviour* of a titanium alloy under friction rather than being a rigorous quantitative study, in all simulations distance, time, velocity, and force were given in units of $l^{(0)}$, M/η, $l^{(0)}\eta/M$, $k_B T/l^{(0)}$, respectively. The model was run for 150 steps. In Figure 1, the temporal evolution of the friction force is depicted, where it was found that equilibrium was attained after a few steps. This behaviour is in agreement with theoretical [6] and experimental observations [8]. For the simulations of Figure 1, the model for strong bonds was considered.

Then, varying the velocity, predictions were obtained for the behaviour of the friction force in the different velocity regimes. As can be seen in Figure 2, there are two sliding regimes (at low and high velocities) with a stick-slip region between them (at intermediate sliding velocities).

The three frictional regimes exhibit different behaviour, with different mechanisms being responsible for the frictional behaviour observed. The low sliding velocity regime represents a state where thermal bond dissociation determines junction fracture rather than shear-induced stress. This regime behaviour correlates with the observation that the value of static friction depends on the time scale. This

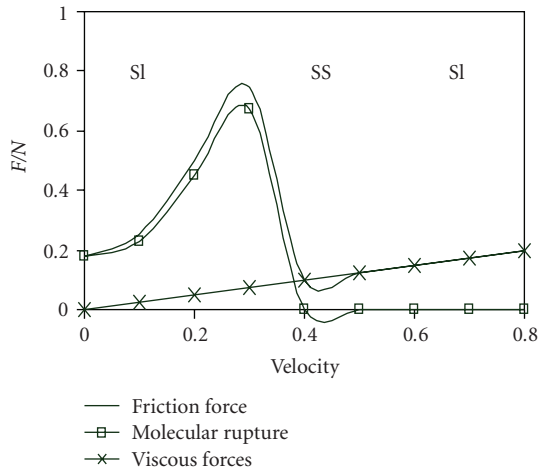

Figure 2: Velocity dependence of frictional forces in the case of strong bonds. The resulting friction force is the collective effect of microscopic bond forces and viscous forces. The symbols Sl and SS indicate sliding and stick-slip regions.

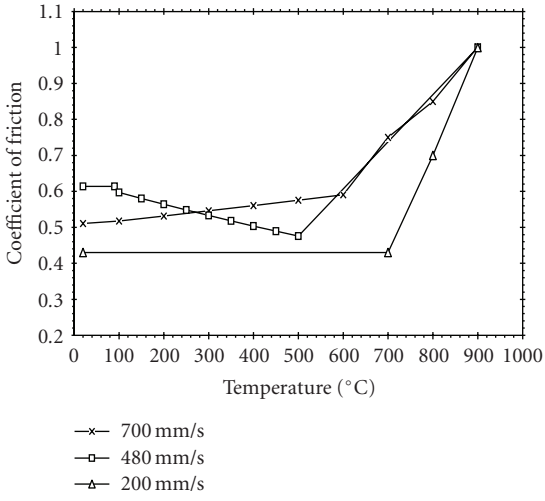

Figure 3: Variation of friction coefficient with temperature at different sliding velocities for Ti6Al4V [8].

region is consistent with atomic scale stick-slip motion of individual junctions. The low sliding velocity frictional regime, which is characterised by energy dissipation, is dependent on the fracture and the subsequent relaxation of junctions, rather than on viscous dissipation, as Figure 2 shows.

In the stick-slip region, at intermediate sliding velocities, the processes of spontaneous and shear-induced bond dissociation compete and produce an erratic stick-slip motion. The stick-slip region has a more regular behaviour as velocity increases. Junction fracture is controlled by the effect of shear stress on the activation barrier. At this time, the fraction of intact junctions decreases with a similar decrease of the fracture contribution to the energy dissipation. The net kinetic friction is relatively insensitive to the sliding velocity in this regime as the effect of the diminishing fractures contribution is counterbalanced by the viscous component of the energy dissipation. The system shows a cooperative behaviour, where as the number of breaking bonds increases, the force on the remaining bonds increases and bond rupture synchronises; thus producing a more consistent stick-slip behaviour. There is a correlation between macroscopic frictional properties and a collective behaviour of microscopic bonds [9].

The high sliding velocity region shows a transition from stick-slip behaviour to smooth sliding. Bond formation becomes impossible due to short-contact times. Frictional force in this regime is completely determined by viscous dissipation.

The results of these simulations are in qualitative agreement with experimental data available for titanium alloy Ti6Al4V (Figure 3, [8]). The frictional behaviour experiments with the titanium alloy were designed and done in such a way so as to measure the coefficient of friction for different parameters of a thin rotating tube under stress. The experimental setup represented accurately the frictional conditions of an ideal solid surface rubbing at a constant velocity against a stationary surface of the same material. As can be seen, for intermediate sliding velocities, friction force decreases with temperature while for low and high sliding velocities friction force increases. As already mentioned, the present work concerns the study of *behavioral trends* of a titanium alloy under friction, hence no direct comparison between the analytical model and the experimental data can be made yet. However, the predicted behaviour by the model seems to agree with the experimental results on the existence of a stick-slip region in the intermediate velocities range.

4. CONCLUSIONS

The mathematical theory of friction is still far from being complete in order to explain the behaviour of materials under friction. For instance, the existing theories of macroscopic friction can not account for frictional behaviour demonstrated during experiments with dry sliding which showed dependence on interface temperature, as well as on rubbing velocity. In this work, an analytical model was employed and applied to titanium alloy Ti6Al4V. The model demonstrated qualitatively a dependence of frictional behaviour on sliding speed, with stick-slip phenomena being responsible for this. The model was found to be in agreement with the theoretically expected and experimentally observed material behaviour [8]. However, the model is not complete yet; as has been shown, the coefficient of friction is not only influenced by velocity variations but by temperature variations as well [8]. It is suggested that the dependence on temperature should be further explored by its incorporation in the analytical contact model, possibly through the material elastic constants, which are known to be temperature-dependent [8]. In this way, appropriate constitutive laws will be developed, which will assist the contact model in more accurately predicting material behaviour under friction and identify the velocity ranges for the various frictional regimes. Currently, work is under way for the derivation of such laws, which will parameterise the frictional behaviour dependence on sliding velocity, as well as interface temperature.

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