Continuum contact mechanics theories at the atomic scale
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Surface roughness, which is always present in some length scales, has a major impact on most tribology-related studies. This is mainly because it can alter the surface forces, which are dominant at the nanoscale, and influence the functionality of micro and nano-sized devices; in fact, contact itself is initiated at the atomic scale. Considering the breakdown of the macroscopic laws of friction at the atomic scale, numerical simulations, such as molecular dynamics (MD), are used to study these systems. Surfaces in nature and engineering applications have random roughness that can be described as being fractal; however, many analytical models, such as those based on the Greenwood-Williamson (GW) model [1], treat roughness as a statistical collection of parabolic asperities.

**Atomic Hertzian Contact**

The Hertz contact theory was examined by studying the pressure distribution of the non-adhesive contact between a number of spherical rigid indenters with different sizes, ranging between 15 Å and 1000 Å, on a deformable atomically flat substrate [4]. The system was generated from calcium atoms, at 300 K.

Contacting system: (Left) A spherical cap indenter of R = 1000 Å indents an atomically flat substrate. The blue, red, green, and white dots represent the fixed, thermostatic, Newtonian, and indenter atoms. (Right) The system’s responses were collected up to the point before which the stress fields were affected by the boundaries.

**Deviations between MD results and Hertz**

Based on the Hertz theory force can be described as:

\[ F_H = \frac{4E^*R^3}{3d^2} \left( \frac{1}{1 + \frac{2E^*}{Rd}} \right), \]

and

\[ R: \text{Indenter’s radius}, \ d: \text{Indentation depth}, \ E^*: \text{Elastic modulus}, \ \gamma_c: \text{Poisson’s ratio}. \]

The applicability of this method was investigated through the pressure distribution at the contacts.

**Pressure distribution at the contact**

(a, b) The interacting atoms were detected by a non-zero pressure criterion. The Hertz formula was fitted to the smoothed data, only after the background noise was removed with a threshold of 0.02 GPa.

(c) The Hertz theory describes the pressure distribution as \( p(x) = p_0(1 - r/c)\gamma_c \gamma_s \), where \( p_0 \) is the maximum pressure, and \( r \) is the contact radius. These values were used for estimating the reduced modulus \( E^* = p_0c \). The results showed that the fitted values of \( E^* \) vary with indentation depth for shallow indentations, and tend toward the reduced Young’s modulus of the material, i.e., \( E^* = 28.57 \) GPa that is calculated based on the employed potential energy. Note that the jaggedness of the results of 15 Å and 20 Å is due to the inevitable stepped geometry of the smaller indenters.

**Redefinition of \( E^* \)**

Based on the results, it is proposed that: \( E^*_{\text{estimated}} = C + AD^2 \), with \( 0 \leq d \leq 4 \) Å, and \( A, B, \) and \( C \) being constants.

Comparisons between the force-indentation curves show the effects of using different values of \( E^* \) for the Hertz theory: Fitted \( E^* \), \( E^*_{\text{estimated}} \), and \( E^*_{\text{constant}} = 28.57 \) GPa.

**Future work**

Future studies will focus on randomly rough surface contacts in dry/lubricated conditions.