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A Numerical Model for Calculation of the Restitution Coefficient of Elastic-Perfectly Plastic and Adhesive Bodies with Rough Surfaces

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Abstract

An in-house contact mechanics model is used to simulate contact of rough spheres having elastic-perfectly plastic contact with adhesion. The model uses a Boundary Element Method (BEM) and employs Fast Fourier Transforms (FFT) for numerical efficiency. We have validated our model for smooth surfaces with the Hertz contact behaviour in elastic regime, JKR adhesive model in the adhesive regime and Thornton and Ning's analytical model in elasto-plastic adhesive regime. Furthermore, the effect of yield stress, interface energy and surface roughness on the Coefficient of Restitution (COR) is investigated. The results show that surface roughness dramatically affects the COR and higher roughness values lead to lower CORs in general. In addition, changes of COR based on different maximum indentation depth in the presence of surface roughness consists of 3 stages; The asperity dominant, bulk elastic dominant and bulk plastic dominant. Interestingly, it was shown that there is a critical indentation depth in which the effect of surface roughness will disappear and rough surfaces act like smooth ones. This critical indentation depth is proportional to the R_q value of the surface roughness. Numerical results suggest that the yield stress influences the COR and higher yields stress results in higher COR for both rough and smooth surfaces. Results also suggest that the effect of interface energy on the COR for smooth surfaces is significant at low indentations and minimum for rough surfaces.

Keywords: Coefficient of restitution; Roughness; Adhesion; Contact mechanics

1 Introduction

Interaction of particles is an important phenomena in the assemblies of particles and their bulk behaviour in a wide range of applications such as food and biosystems [1], pharmaceuticals [2], rock mechanics [3] and gas particle flows [4]. The collision between particles have been extensively studied analytically [4], numerically [5] and experimentally [6]. In terms of the elastic contact, Hertzian contact model has been widely used which offers a non-linear

32 behaviour [7, 8]. However, in majority of the granular flow simulations simple linear model is
33 used to increase the computational efficiency. Since different materials show complicated
34 plastic behaviours, incorporation of a complete analytical model for elasto-plastic contact is a
35 challenge. Therefore semi-analytical models are often used to account for the effect of
36 plasticity in contact mechanics [9]. Other works have introduced simplified linear models using
37 Finite Element Analysis (FEA) [10, 11]. These models can be used to numerically and
38 analytically calculate the COR based on the loading and unloading energy.

39 It was shown that adhesion is playing an important role in the dissipation of the contact energy
40 and the coefficient of restitution and several theories were introduced [12]. In an analytical
41 model developed by Thornton and Ning [4] coefficient of restitution was modelled for an
42 elasto-plastic contact with consideration of adhesion. The model showed that coefficient of
43 restitution is dependent on the impact velocity, yield stress and the interface energy. Analytical
44 and semi-analytical models are easy to implement numerically, however they do are not able
45 to take into account the complexities that real engineering surfaces could have such as surface
46 roughness. The effect of surface roughness in the contact mechanics have been the subject of
47 many studies. The pioneering work of Greenwood and Williamson (GW) [13] has shown that
48 the surface roughness can influence the real area of contact and the discrete contact pressures.
49 The theory assumed a distribution of the surface asperity height with similar geometry and
50 asperity radius and the interaction of individual asperities was ignored in the model. Following
51 that, numerous works have considered the effect of surface roughness in solving the contact
52 problems [14-16]. Others used half-space approximation and numerous mathematical models
53 for increasing the efficiency of the computations [17-19]. More recently, researchers developed
54 models for the elasto-plastic contact of rough surface [20-22]. Recent advances in
55 computational power and contact algorithms led to development of contact mechanics models
56 with finer grids and consideration of adhesive problems [23-25]. Surface roughness is known
57 to alter the loading and unloading behaviour of materials, therefore affecting the energy
58 dissipation. It also dramatically affects the separation of surfaces, real area of contact and
59 adhesion. Hence, importance of the surface roughness in calculation of energy dissipation and
60 restitution coefficient is clear.

61 Despite the fast improvements in simulating the contact mechanics of real engineering surfaces,
62 to the best of authors' knowledge, very scarce numerical models of granular materials consider
63 the roughness as an input parameter. Recently attempts have been made to consider the effect
64 of roughness on the normal force-displacement of particulate solids [26-28]. However, the

65 effect of surface roughness on calculation of COR is still not studied numerically. Interestingly,
66 this has only been studied experimentally to investigate the effect of roughness on wettability
67 and COR in butterfly wings [29]. In this paper, a numerical in-house BEM contact mechanics
68 model that considers elastic-perfectly plastic and adhesive contact of rough surfaces have been
69 employed to calculate the COR. The theory of the model as well as its validation have been
70 presented in Section 2. The effect of surface roughness, yield stress and interface energy (to
71 take account of adhesion) on the COR has been reported in Section **Error! Reference source**
72 **not found..** The results of the current model, for the first time, highlight the importance of
73 surface roughness in determining the COR in particle-particle interactions.

74 **2 Theory**

75 **2.1 Elastic-perfectly plastic contact**

76 The normal force-displacement relationship for the contact of rough particles is modelled using
77 our contact mechanics in-house code [30]. In the case of contact of rough surfaces, only highest
78 asperities of surfaces will stand the load and the area of real contact is orders of magnitude
79 smaller than the nominal contact area. The contact mechanics model is a coupled model in
80 which load on any asperity can deform the whole material with respect to the influence
81 coefficients [7]. The problem is to solve the complementary potential energy in order to obtain
82 the true stress and strain matrices. The composite deformation of the surfaces $u(x, y)$ due to
83 the applied load of $p(x, y)$ can be calculated by the linear convolution according Boussinesq-
84 Cerruti theory:

$$85 \quad u_e = K * p_d = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} K(x - \xi, y - \eta) p(\xi, \eta) d\xi d\eta \quad (1)$$

86 in which x and y are two dimensional coordinates, K is the convolution kernel and can be
87 calculated from the half-space approximation as the following:

$$88 \quad K(x - \xi, y - \eta) = \frac{1}{\pi E^*} \frac{1}{\sqrt{(x - \xi)^2 + (y - \eta)^2}} \quad (2)$$

89 where E^* is the composite elastic modulus of both materials $(\frac{1}{E^*} = \frac{(1-\nu_1^2)}{E_1} + \frac{(1-\nu_2^2)}{E_2})$.
90 Here, ν_1, ν_2, E_1 and E_2 are the Poisson's ratio and Elastic Modulus of material 1 and 2
91 respectively. For the sake of numerical calculations efficiency, roughness of both surfaces can
92 be integrated as a composite surface roughness only on one contacting surface and the counter-
93 body can be assumed to be rigid [7]. Therefore, by movement of the rigid body in normal

94 direction, the body interferences (i) are calculated as shown in Figure 1. For the points of
 95 contact, the elastic deformation calculated using Equation 1 should be equal to the body
 96 interference (i). In order to solve the contact problem numerically, the load balance also should
 97 be considered. This will imply that the sum of all nodal contact pressures should equate the
 98 total normal applied load. The model considers a perfectly plastic behaviour and a yield criteria
 99 is assumed to be the cut-off value for the contact pressure at every node. The surface asperities
 100 that reach the yield pressure are assumed to float freely on the surface and do not take part in
 101 the deformation calculations. Therefore, the set of the following equations should be solved
 102 iteratively.

$$\left. \begin{array}{l}
 r = (Z_2(x, y) - Z_1(x, y)) + \overline{u_z}(x, y) \quad \forall x, y \in A_c \quad (3.1) \\
 p(x, y) > 0 \quad \forall x, y \in A_c \quad (3.2) \\
 p(x, y) < p_y \quad (3.3) \\
 \sum_{i,j=1}^{i,j=N} p_{i,j} = F_N \quad (3.4)
 \end{array} \right\} \quad (3)$$

104 In Equation 3 r is the rigid body movement of two rough surfaces in normal direction, Z_2 and
 105 Z_1 are the surface profiles of the two rough particles and $\overline{u_z}$ is the composite elastic deformation
 106 of two materials calculated by Equation 1. F_N is the total applied load in the normal direction,
 107 p_y is the yield stress of the softer material in contact, A_c is the area of contact and N is the total
 108 number of nodes in the domain of study. In the current contact mechanics model, an elastic-
 109 perfectly plastic approach is incorporated. Yield stress of the softer material is set to be the
 110 threshold for the plastic flow and the pressure does not exceed this value. This approach is
 111 widely used in other works in order to simulate elastic-plastic contacts. More details of the
 112 contact mechanics approach can be found in Refs [31, 32].

113 2.2 Adhesion

114 The model for adhesive contact of smooth surfaces was developed by Johnson et al. [33] (JKR)
 115 where they extended the Hertzian contact to account for adhesive region. There have been
 116 numerous attempts to adapt JKR theory to different applications [34, 35]. In recent years,
 117 development of numerical models for adhesive contact of rough surfaces have been the subject
 118 of many studies [23, 36-38]. The BEM model developed by Pohrt and Popov [39, 40] was used
 119 in this work which introduced a local mesh size-dependant criteria for detachment of surface
 120 asperities in adhesion.

121 In the adhesive contact the first part of Equation 3 will be modified as:

122
$$r = (Z_2(x, y) - Z_1(x, y)) + \overline{u_z}(x, y) + d \quad (4)$$

123 in which d is the pulled apart distance (Figure 2) when surfaces are unloading. It should be
 124 noted that the surface stresses that only occur inside the contact region for non-adhesive
 125 contacts are positive (compressive). When the bodies keep the same contact area after
 126 compression and are pulled away for a distance d , Equation 4 will be valid. Therefore, set of
 127 Equation 3 will be solved iteratively but the first part is replaced with Equation 4. It should be
 128 noted that the adhesive forces are considered in both loading and unloading. In order to consider
 129 adhesion in loading, after each loading step, a small unloading step ($d=0.1$ nm) was considered.
 130 The local detachment criteria was then applied as the following [39]:

131
$$p_d = \sqrt{\frac{E^* \Delta\gamma}{0.473201 \cdot h}} \quad (5)$$

132 $\Delta\gamma$ is the interface energy and h is the grid size. Equation 5 calculates the maximum tensile
 133 (adhesive) pressure that a node can sustain before detachment. If the tensile stress at each node
 134 exceed the p_d value, the detachment occurs and the stress will be set to zero.

135 **2.3 Numerical discretisation**

136 In order to solve the set of Equations 3, the numerical domain should be discretised into
 137 rectangular elements of similar size in which the contact pressure can be assumed to be
 138 constant. Equation 1 will get the discretised form given by:

139

140
$$u_{(i,j)} = K * p_d = \sum_{k=1}^N \sum_{l=1}^N K(i-k, j-l) p(k, l) \quad i, j = 1, 2, \dots, N \quad (6)$$

141 where $p(k, l)$ is the constant pressure acting on the element centred at (k, l) . Solving Equation
 142 6 along with Equation 3 requires an iterative process to modify the contact pressures and
 143 finding the corresponding surface deformations. This can be solved using the matrix inversion
 144 process and requires $N^2 \times N^2$ operations. Using DC-FFT algorithm widely reported in the
 145 literature [17, 41, 42] can reduce the computational demand dramatically. Equation 6 will be
 146 then converted to:

147
$$u_{(i,j)} = IFFT[\tilde{K}_{i,j} \cdot \tilde{p}_{i,j}] \quad i, j = 1, 2, \dots, N \quad (7)$$

148 where $\tilde{K}_{i,j}$ and $\tilde{p}_{i,j}$ are the Fast Fourier Transforms (FFT) of the influence coefficient and
 149 contact pressure matrices and are multiplied element-by-element. The FFT-based convolution
 150 is accompanied by periodicity errors that can be minimized by means of zero-padding contact
 151 pressure matrix (doubling the domain and putting zero pads in both x and y directions) and
 152 wrap-around [41]. It should be noted that dealing with 2-dimensional surfaces, both contact
 153 pressure and influence matrices should be expanded in both x and y directions. In order to
 154 increase the applicability and efficiency of the method, the number of nodes chosen for the
 155 numerical study should be a power of 2. The surfaces used in this study consist of 512×512
 156 nodes of 0.25 μm size for 500 μm radius spheres.

157

158 **2.4 Calculation of the COR**

159 It should be highlighted that parameters such as impact angle and tangential loading or friction
 160 have significant impact on the energy dissipation and the COR. In this model only the normal
 161 impact of the particles has been considered. Considering other parameters such as tangential
 162 stiffness will add more complexity to the model and can be the subject of future studies. Once
 163 the contact behaviour of loading and unloading is modelled, calculation of the COR will be
 164 straightforward by simply calculating the energy of loading and unloading from the area under
 165 the curve in load-displacement graph. The formula for the calculation of COR will be as the
 166 following:

$$167 \quad COR = \sqrt{\frac{W_u}{W_l}} \quad (8)$$

168 In Equation 8, W_l is the energy of loading that is transferred to the material and W_u is the energy
 169 which is released from the material in the process of unloading. The calculation of W_l and W_u is
 170 shown schematically in Figure 3.

171 **2.5 Numerical model validations**

172 2.5.1 Hertzian contact

173 An example of the surfaces used in the numerical simulation is shown in Figure 4. In order to
 174 obtain the normal force-displacement curves, the upper particle (upper surface) is moved in the
 175 normal direction. The normal force (F_N) is then calculated from the contact mechanics code
 176 solving the set of Equation 3. Movement of the upper surface is adjusted by changing the value

177 of r in Equation 3. The indentation of the particles is simulated with step-wise increase in the
178 value of r and the corresponding normal force is recorded. The results of normal force-
179 displacement is compared with the Hertzian model for the case of smooth particles with $500\mu\text{m}$
180 radius, Young's modulus of 210 GPa (resembling a typical grade of steel) and Poisson's ratio
181 of 0.25 in Figure 5 in order to test the accuracy of the elastic numerical model prior to elasto-
182 plastic and adhesive simulations. It should be noted that the shape of surface asperities
183 influence the calculation of the real contact area and the corresponding surface pressures (this
184 is still an open area of research in the field of contact mechanics [25]). Consideration of other
185 properties of rough surfaces such as slope of the surface roughness in the calculation of surface
186 area, energy dissipation and COR will be the subject of future developments of the model.

187 2.5.2 Elastic-perfectly plastic contact

188 The same numerical approach as the previous section has been implemented with incorporation
189 of the yield cut-off (Equation 3.3). It is assumed that the loading occurs in elastic-perfectly
190 plastic mode and the unloading is only elastic. The loading and unloading of particles have
191 been simulated and the results are compared to the analytical model of Thornton and Ning [4].
192 The simulations were conducted for two smooth spheres of $500\mu\text{m}$ radius with elastic modulus
193 of 210 GPa and Poisson's ratio of 0.25. The yield pressure was set to 750MPa. Numerical BEM
194 simulations were carried out for surfaces of $125\mu\text{m}\times 125\mu\text{m}$. BEM numerical results of Figure
195 6 show very good agreement with the prediction from analytical model of Thornton and Ning
196 [4].

197 2.5.3 Adhesive contact

198 Adhesion was considered in both loading and unloading and for validation purposes, the
199 adhesive contact was simulated for the unloading of surfaces using the theory of Pohrt et al.
200 [39] by step-wise increasing of parameter d in Equation 4. It should be noted that the resolution
201 in the z direction is 0.1nm in our simulations. All the simulation parameters are the same as the
202 elastic model shown earlier (elastic modulus of 210 GPa and Poisson's ratio of 0.25). The
203 interface energy ($\Delta\gamma$) in the range of 0.01 to 0.09 ($\frac{J}{m^2}$) is used in Section 2.5.5 of this
204 manuscript for comparison reasons. However, in this section and other simulations, the highest
205 value 0.09 ($\frac{J}{m^2}$) is selected to signify the effect of adhesion on the COR for both rough and
206 smooth surfaces. The formulation of the JKR theory has been taken from [39]. The critical
207 point that the maximum adhesive force will occur for a parabolic profile is formulated as the
208 following:

209
$$F_{adh} = \frac{3}{2} \Delta\gamma\pi R \quad (9)$$

210
$$a_c = \left(\frac{9\pi \Delta\gamma R^2}{8 E^*} \right)^{\frac{1}{3}} \quad (10)$$

211
$$d_c = - \left(\frac{3\pi^2 \Delta\gamma^2 R}{64 E^{*2}} \right)^{\frac{1}{3}} \quad (11)$$

212 F_{adh} is the total normal force required to separate the surfaces, a_{crit} is critical value of the
 213 contact radius at the moment of detachment and d_c is the crucial value of the negative
 214 indentation at the time of detachment. For comparison reasons, normalized indentation (\bar{d}),
 215 normalized force (\bar{F}) and the normalized area (\bar{a}) are formulated as:

216
$$\bar{d} = 3\bar{a}^2 - 4\bar{a}^{\frac{1}{2}} \quad (12)$$

217
$$\bar{F} = \bar{a}^3 - 2\bar{a}^{\frac{3}{2}} \quad (13)$$

218
$$\bar{F} \approx 0.12(\bar{d} + 1)^{\frac{5}{3}} - 1 \quad (14)$$

219

220 The results of simulation for elastic adhesive contact are plotted in Figure 7 and compared
 221 with the JKR theory, where a good agreement can be observed.

222 2.5.4 Effect of yield stress

223 Simulations were conducted at different yield stress values of 0.75 and 1.5 GPa for adhesive
 224 contact ($\Delta\gamma = 0.09 \frac{J}{m^2}$) of two smooth spheres. All other simulation parameters (radius,
 225 Young's modulus and Poisson ratio) are kept the same as the previous section. The results are
 226 plotted in form of COR (Equation 8) as a function of indentation depth in Figure 8. In order to
 227 compare the results with the analytical model of Thornton and Ning [4], the impact velocity in
 228 their work has been converted to the indentation depth by using the energy equations:

229
$$\frac{1}{2} mV^2 = \int F \cdot di \quad (15)$$

230 In the energy equation above, V is the impact velocity, m is the mass of the particle, F is the
 231 total normal force and di is the incremental indentation until the maximum indentation reaches.

232 It can be seen that the results are following similar trends as reported by Thornton and Ning
233 [4], where for both yield stresses the COR initially increases by the indentation and then
234 reduces.

235 2.5.5 Effect of interface energy

236 Interface energy is known to affect the adhesive force and thus the COR. Simulations were
237 carried out for smooth surfaces for different values of interface energy from $\Delta\gamma =$
238 $0.01(\frac{J}{m^2})$ to $0.09(\frac{J}{m^2})$, but constant yield stress of 750 MPa. The results are plotted in Figure
239 9 in log scale in order to make the difference clear. Results suggest that interface energy only
240 affects the COR at small indentations where the effect of adhesion is comparable to elastic and
241 plastic energies. The findings are in-line with the findings of Thornton et al. [4] which used
242 higher values for the interface energy. In this paper, we have chosen a range for the interface
243 energy that are mostly observed in the engineering applications.

244 **3 Effect of Root Mean Square surface roughness**

245 Calculation of the contact behaviour of the rough surfaces is carried out using the theory
246 presented in Section 2, considering the initial digital topography input of the model. The
247 discretisation procedure of the rough surface topography is also discussed in Section 2.3.
248 Rough surfaces are generated incorporating the method introduced by Hu et al. [43] who used
249 2-D digital filters and autocorrelation functions. Fast Fourier Transforms are used for
250 numerical efficiency. There are several parameters that can be used to characterise the
251 topography of the surfaces such as Root Mean Square (RMS) roughness, Skewness, kurtosis
252 etc. Incorporation of all these surface parameters in a digitised surface needs a careful
253 characterisation of the real engineering surfaces and extracting the desired parameters as input
254 to the surface generation models [44]. Therefore, for simplicity, generation of rough
255 topography was carried out by only introducing the RMS roughness of the surfaces (R_q). The
256 topography was generated off-line prior to any contact calculations and used as input for the
257 contact solver. Surfaces used in the model are similar to the ones shown in Figure 4. The upper
258 surface is set to be perfectly smooth and the lower surface has the composite surface roughness
259 of both particles in contact. The contact in this condition is known to be equivalent to the real
260 system of two rough particles. The effect of surface roughness on the COR of an elasto-plastic
261 adhesive contact (elastic modulus of 210 GPa, yield pressure of 750MPa and Poisson's ratio
262 of 0.25) have been studied numerically and the results are plotted against the maximum
263 indentation depth in Figure 10.

264 The maximum indentation depth is the depth that loading is stopped and the spheres start to
265 unload. Since the contact mechanics algorithms inevitably use indentation depth and numerical
266 simulations are based on this concept, it is more convenient to use the indentation depth as the
267 analysis factor. More importantly, it should be noted that, analysis of rough surfaces should
268 mainly be carried out based on indentation depth since it makes it possible to compare that with
269 the R_q of roughness surfaces. Due to the non-linear behaviour of load and indentation,
270 correlating incident velocity and indentation -and as a result- incident velocity and surface
271 roughness will be highly non-linear and extracting useful information in this stage of the
272 research will be cumbersome.

273 All other simulation parameters are set the same as Section 2.5.2 and Section 2.5.3. For smooth
274 surfaces, COR increases with the maximum indentation depth due to the decreased effect of
275 interface energy. Then a decrease in the COR is observed which is a result of plastic energy
276 dissipation. Results for the smooth case, are in good agreement with the analytical work
277 reported by Thornton et al. [4] in terms of the trend seen. The scenario changes when surface
278 roughness is introduced to the contact.

279 **4 Discussion**

280 From results in previous sections, it can be observed that surface roughness can dramatically
281 influence the COR. There are three distinctive stages in this case. In the first stage, the COR
282 decreases in the beginning and that is due to the initial plastic deformation of asperities. In the
283 second stage, a general increase in the COR is observed which can be due to the reduction in
284 the influence of surface roughness on the overall contact behaviour as the asperities flatten
285 [28]. Finally, a gradual decrease in the COR is observed which is similar to the smooth case
286 and can be attributed to the plastic deformation of the bulk of particle. For the case of $R_q=0.1$
287 μm and $R_q=0.2 \mu\text{m}$ this final decrease is happening earlier than the case of $R_q=0.5 \mu\text{m}$ and $R_q=1$
288 μm and not surprisingly they show a closer behaviour to the smooth surface. Interestingly the
289 values of COR tend to converge to the values for smooth case at certain indentation depths as
290 shown by the arrows in Figure 10. This new finding suggests that in the incident of the rough
291 particles and the corresponding COR, there is a critical indentation depth (i_{cr_max}) in which
292 the behaviour of the rough particles align with the behaviour of smooth particles. The effect of
293 surface roughness on the COR will disappear after the critical indentation depth (i_{cr_max}).
294 This suggest that COR -or energy dissipation in other words- are influenced by the surface
295 roughness mainly where the compression is in the scale of surface roughness, otherwise they

296 tend to be close to the values of smooth surfaces. We have plotted the critical indentation depth
 297 (i_{cr_max}) against normalised surface roughness values (R_q/R) where R is the radius of particles
 298 and the results are shown in Figure 11, where a linear dependency of i_{cr_max} on the R_q/R value
 299 of the surface roughness can be observed. Moreover, as the indentation gets smaller, typically
 300 less than 50nm, the COR for all roughness values follows exactly the same trend, as in this
 301 region plasticity is not dominant. Finally, COR merges to that of a smooth surface below the
 302 indentation of 8nm, regarded as the minimum critical indentation depth (i_{cr_min}), a unique
 303 number for all roundness values. This is where the indentation gets small enough so that only
 304 tip of the first asperities come into contact. The effect of different asperity lateral sizes and
 305 slope of surface roughness will be studied on this phenomena in the future works of the author.

306 It is useful to analyse the energy loss due to surface roughness to highlight its significance. For
 307 comparison reasons, the percentage differences between COR values in the case of smooth
 308 surface and the case of rough surfaces ($(COR_{smooth} - COR_{rough})/COR_{smooth}$) have been calculated
 309 and plotted in Figure 12. The energy dissipation due to roughness can be interpreted based on
 310 the difference shown in Figure 12. The differences in COR are not quantitatively representing
 311 the energy loss, but since COR is equal to $\sqrt{\frac{W_u}{W_t}}$, higher decrease in its value means an increase
 312 in the energy loss. Rougher surfaces show higher deviation from the behaviour of smooth
 313 surfaces for longer indentation depths therefore show higher energy losses.

314 4.1.1 Effect of yield stress and roughness

315 In order to investigate the effect of yield stress on the COR for an adhesive ($\Delta\gamma = 0.09 \frac{J}{m^2}$)
 316 rough surface, simulations were carried out for the surface with $R_q = 0.1\mu m$ for two different
 317 values of yield stress (150 MPa and 750 MPa) and the results are presented in Figure 13. Similar
 318 to the results of Section 2.5.4, it can be seen that yield stress dramatically affects the COR also
 319 for rough surfaces. In the very initial stage of indentation (less than 50nm) where the plasticity
 320 is not yet dominant the trends are similar but a clear differentiation can be observed when the
 321 plastic deformation takes place. The trend emerges to that of a smooth particle beyond the
 322 critical indentation, where plasticity undergoes to a bulk dominant stage.

323 4.1.2 Effect of interface energy and roughness

324 The effect of interface energy on the COR for smooth surfaces has been investigated and
 325 reported in Section 2.5.5. In this section, the effect on the COR for rough surfaces is presented.
 326 Computational results for COR at two different surface energies $\Delta\gamma =$

327 $0.01 \left(\frac{J}{m^2}\right)$ and $0.09 \left(\frac{J}{m^2}\right)$ for the rough surface with Young's modulus of 210 GPa, yield stress
328 of 750 MPa and $R_q = 0.1 \mu\text{m}$ are plotted in Figure 14. Results suggest that interface energy and
329 therefore adhesion have less effect on the loading and unloading behaviour and the
330 corresponding COR for rough surfaces. This is in line with other works in the literature [23,
331 45, 46] that state, interface energy will be dramatically reduced for rough surfaces especially
332 where roughness is significantly larger than the atomic distances due to the large separation of
333 surface points. However, when the surfaces are smooth (Figure 9), interface energy has
334 significant effect on the COR, but only in the regions where plasticity is not dominant.

335 **5 Conclusions**

336 In this work elastic-perfectly plastic and adhesive contact behaviour of surfaces has been
337 simulated using a fast numerical Boundary Element Model (BEM). Coefficient of Restitution
338 (COR) was calculated by considering the loading and unloading energies of smooth and rough
339 surfaces and the following conclusions are drawn.

- 340 - It is shown that BEM is an efficient deterministic method to model the particle contact
341 behaviour and the corresponding loading/unloading curves.
- 342 - For rough surfaces a significant dependency of COR on the surface roughness has been
343 observed. This is the first time that surface roughness has been considered in the
344 numerical calculation of the COR by means of BEM.
- 345 - Our results show that higher values of R_q roughness result in lower COR for the same
346 maximum indentation. This is because higher roughness leads to a greater energy
347 dissipation and thus lower COR. However, this behaviour changes beyond a maximum
348 critical indentation depth (i_{cr_max}) after which COR trend is similar to that of smooth
349 surfaces. This was argued to be where the indentation is beyond the scale of surface
350 roughness and the contact becomes bulk-dominant.
- 351 - It is also found that, below a minimum critical indentation (i_{cr_min}), where the
352 behaviour is mostly elastic, rough surfaces behave similar to that of smooth surfaces.
- 353 - It has been shown that for rough surfaces, the effect of yield stress on COR is
354 significant. The lower yield stress results in lower COR, but only in the regions where
355 the plasticity is dominant.
- 356 - Unlike smooth surfaces, interface energy slightly affects the COR of rough surfaces but
357 in the small indentation regions where the behaviour is more elastic. Therefore, the

358 effect of interface energy on COR for rough surfaces is minimal, due to larger
359 separations of surface points for rough surfaces.

360 Authors believe that consideration of the surface roughness in the bulk behaviour of the
361 granular materials as well as particle-particle interactions is significantly important and will
362 influence the future calculations. The method is fairly fast and could be used for a variety of
363 materials and complicated surface geometries.

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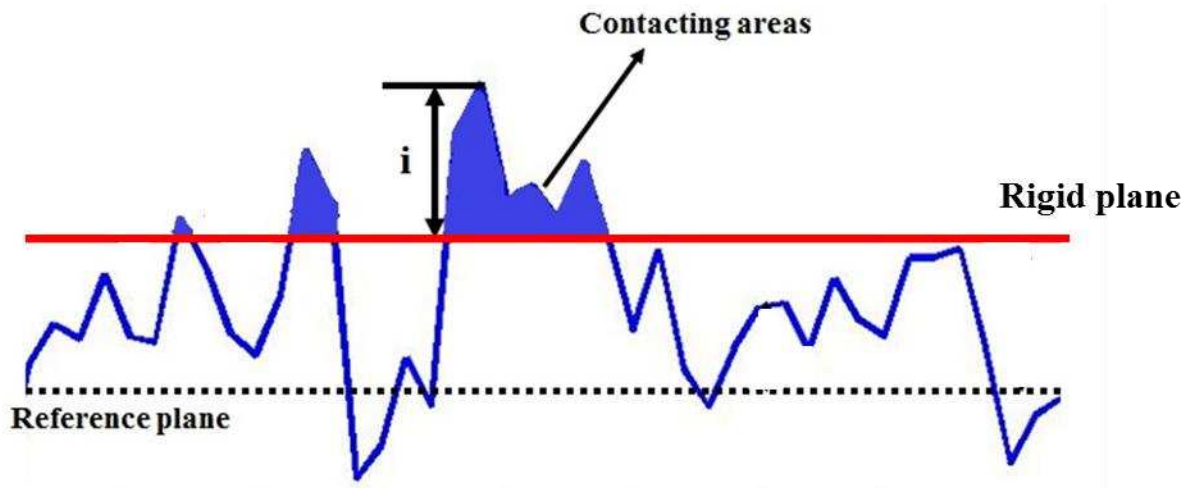
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483 Figure 1 Schematics of the rigid body interference with the composite surface roughness

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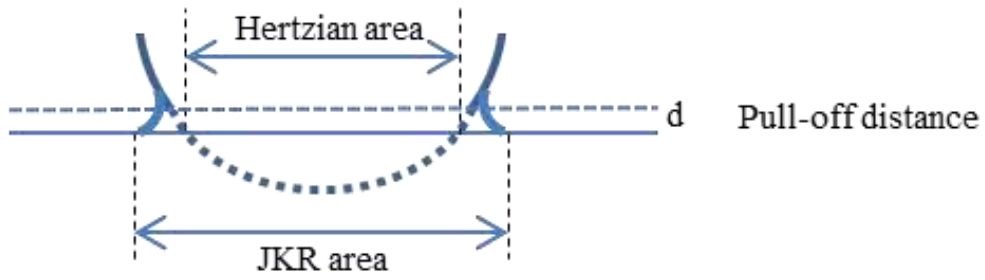
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503 Figure 2 Illustration of the contact geometry based on JKR and Hertzian theory and the pull-
 504 off distance d . Positive (compressive) pressures occur in Hertzian region and repulsive forces
 505 are at the outer ring (JKR region). d is the distance in which surfaces are pulled apart.

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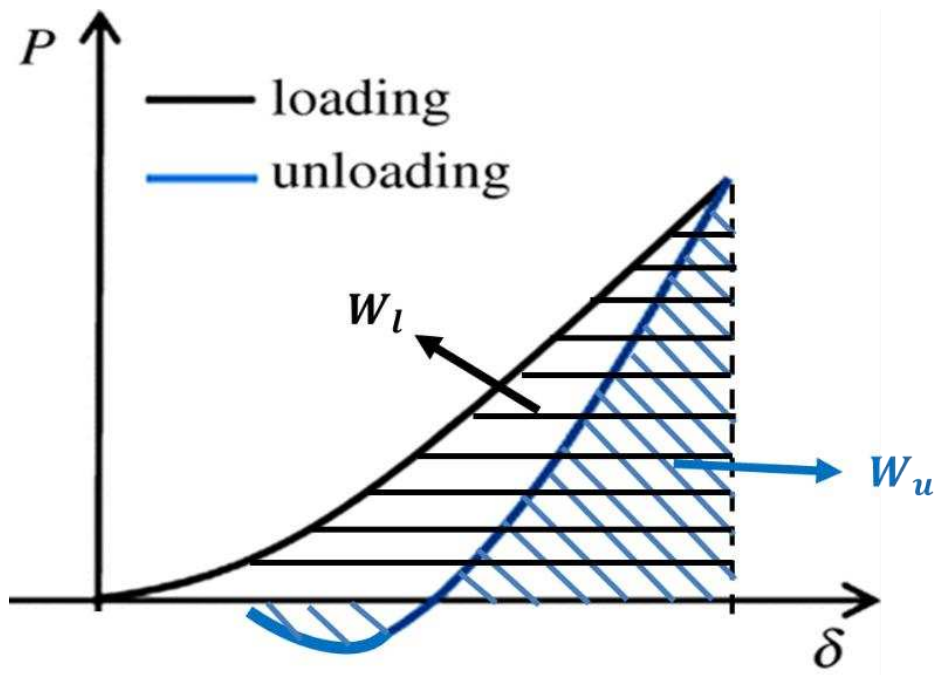
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Figure 3 Schematics of loading and unloading energy calculations

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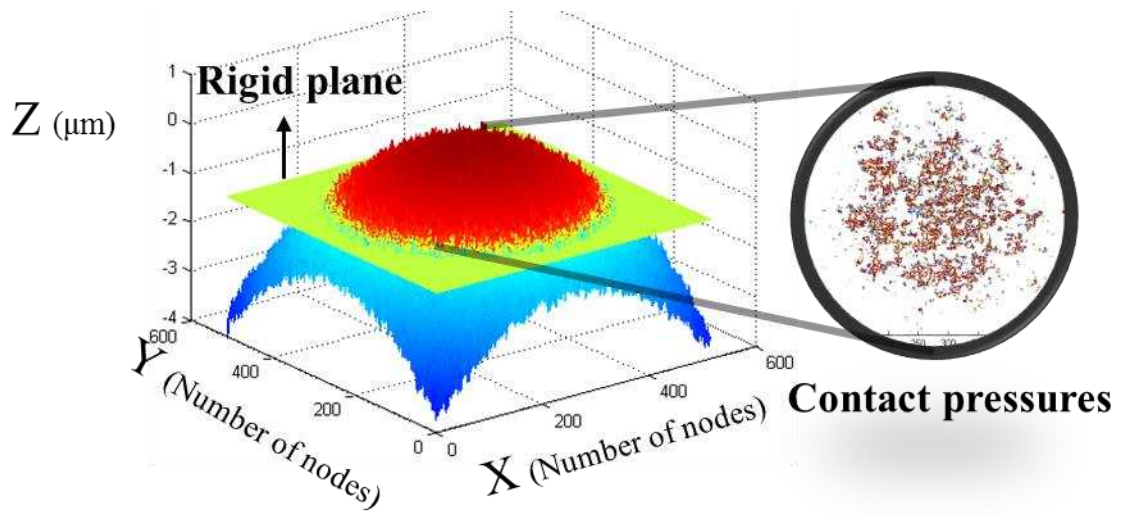
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545 Figure 4 Digitised surfaces, domain, configuration of the BEM and the contact pressures

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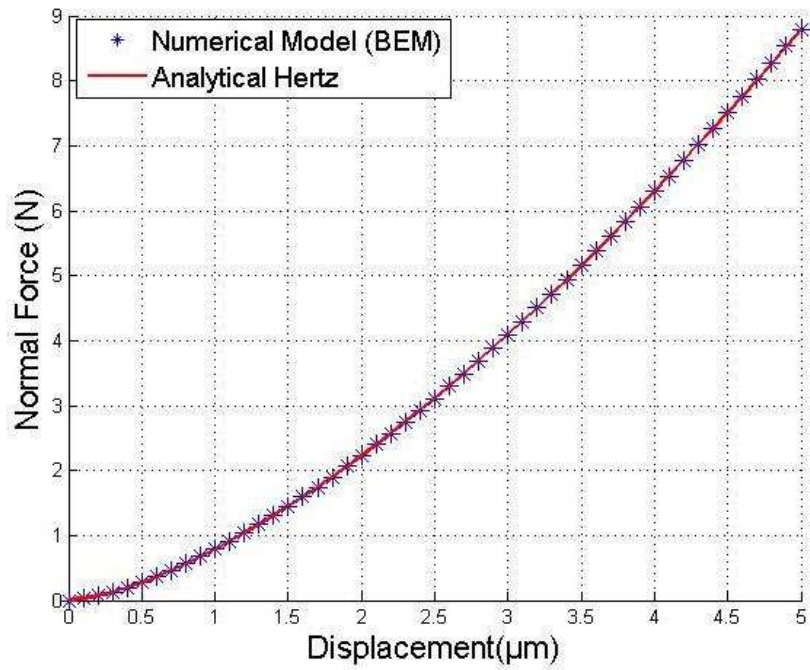
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565 Figure 5 BEM numerical solution of the elastic contact compared with the Hertzian solution

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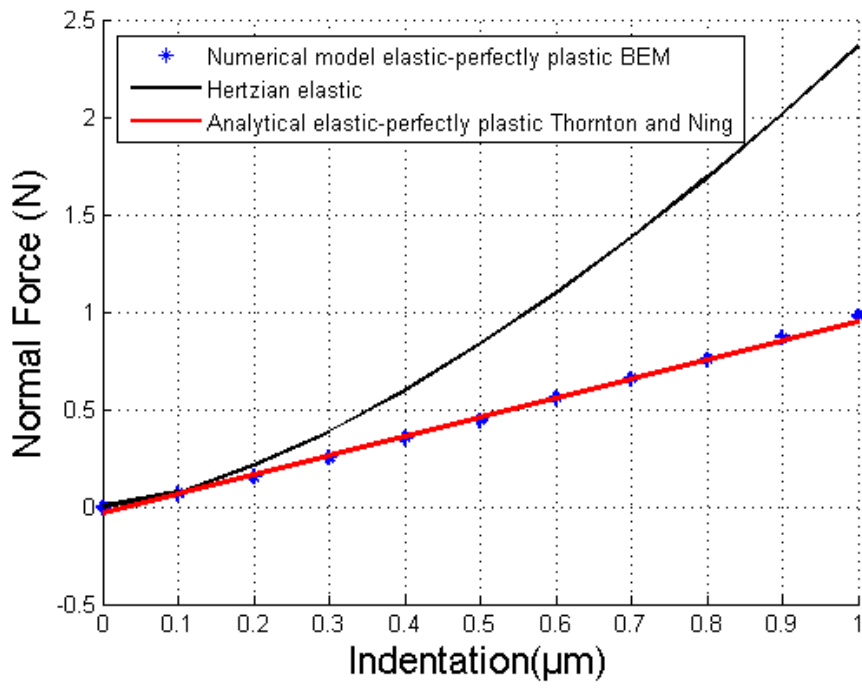
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Figure 6 Comparison of different loading models

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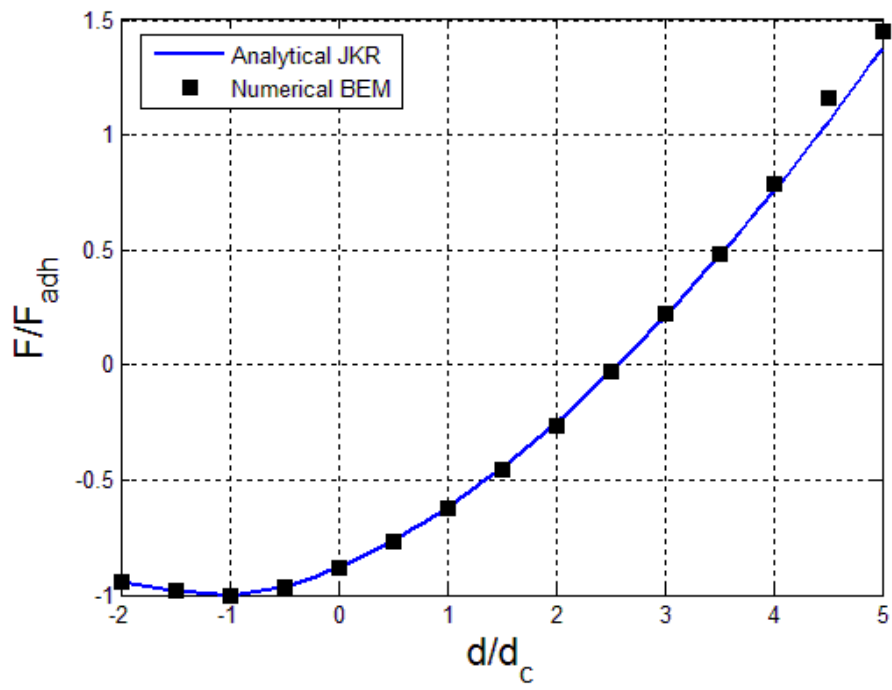
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Figure 7 Adhesive pull-off for the contact of two spheres and comparison with JKR

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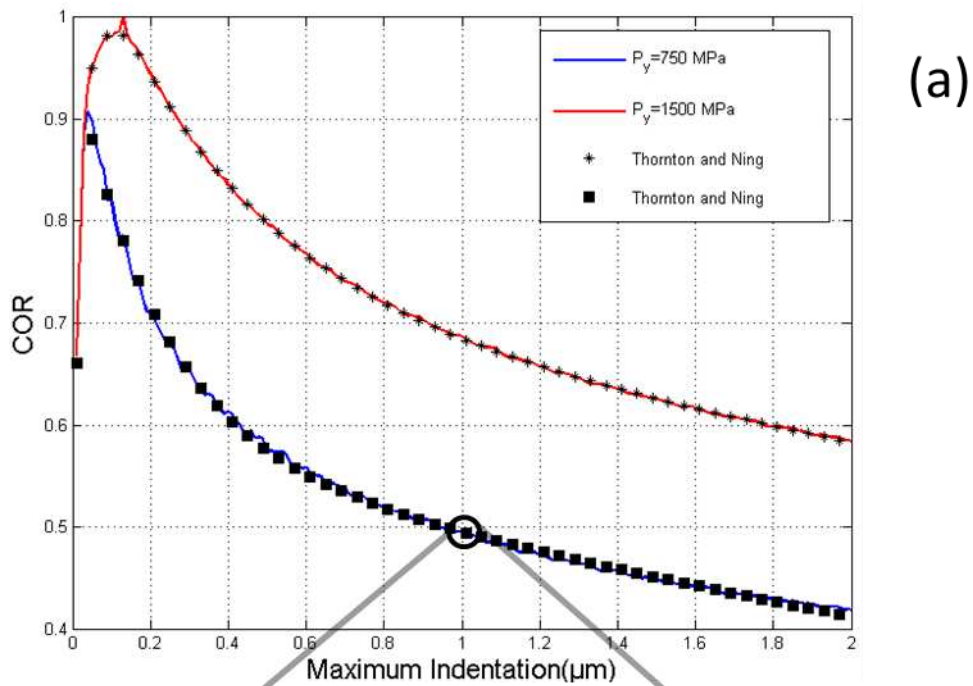
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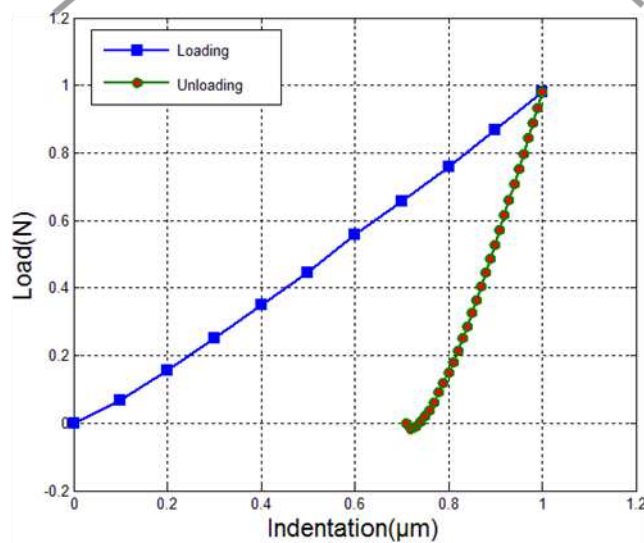
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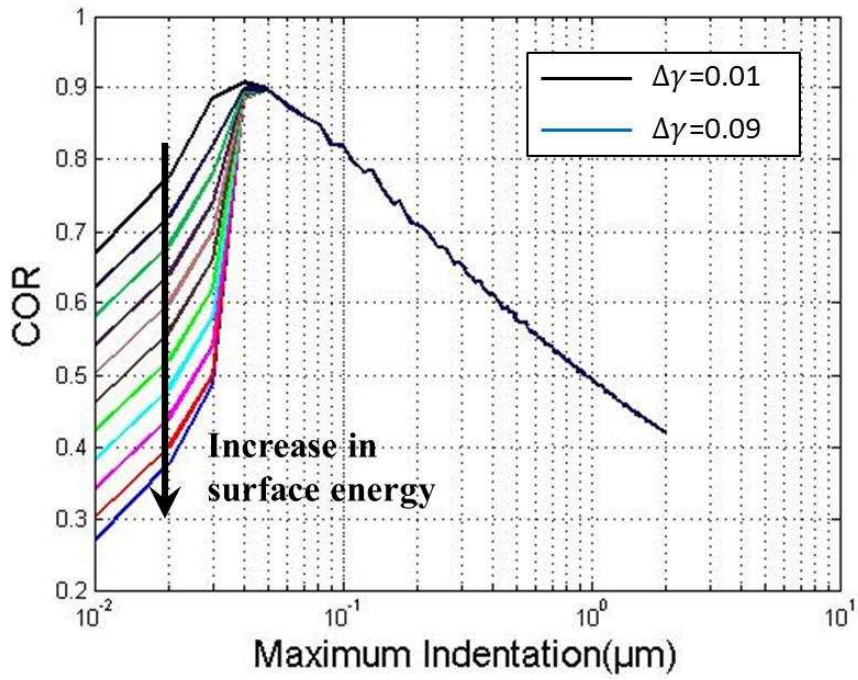
(b)

619 Figure 8 (a) Effect of yield stress on the COR for constant E (210 GPa) and $\Delta\gamma$ ($0.09 \frac{J}{m^2}$)

620 (b) one example of loading and unloading curve for elastic-perfectly plastic and adhesive

621 contact of smooth surfaces at maximum indentation depth of 1 μm for yield stress of 750

622 MPa.



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627 Figure 9 Effect of surface energy on the COR for $\Delta\gamma = 0.01$ to $0.09 \left(\frac{J}{m^2}\right)$ but constant E

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(210 GPa) and yield stress (750 MPa)

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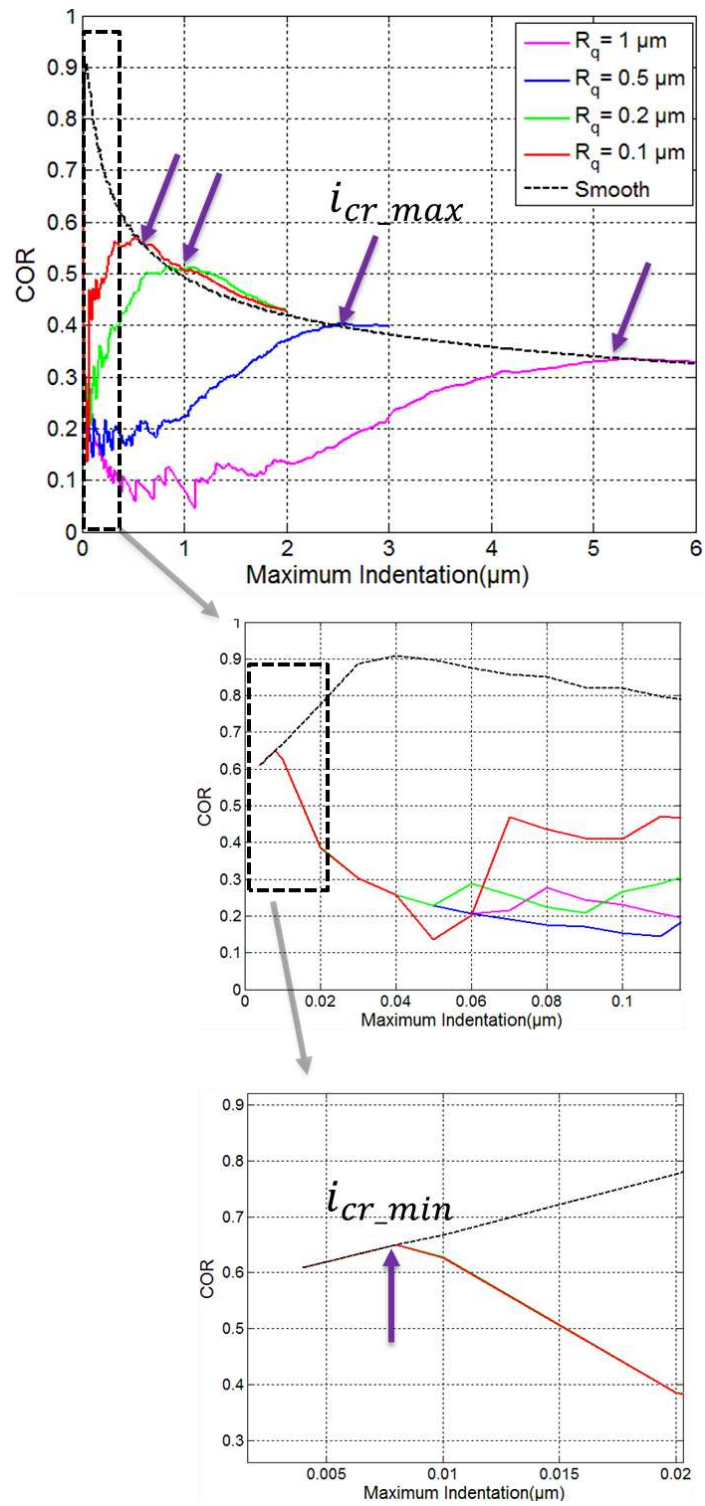
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Figure 10 Effect of surface roughness on COR

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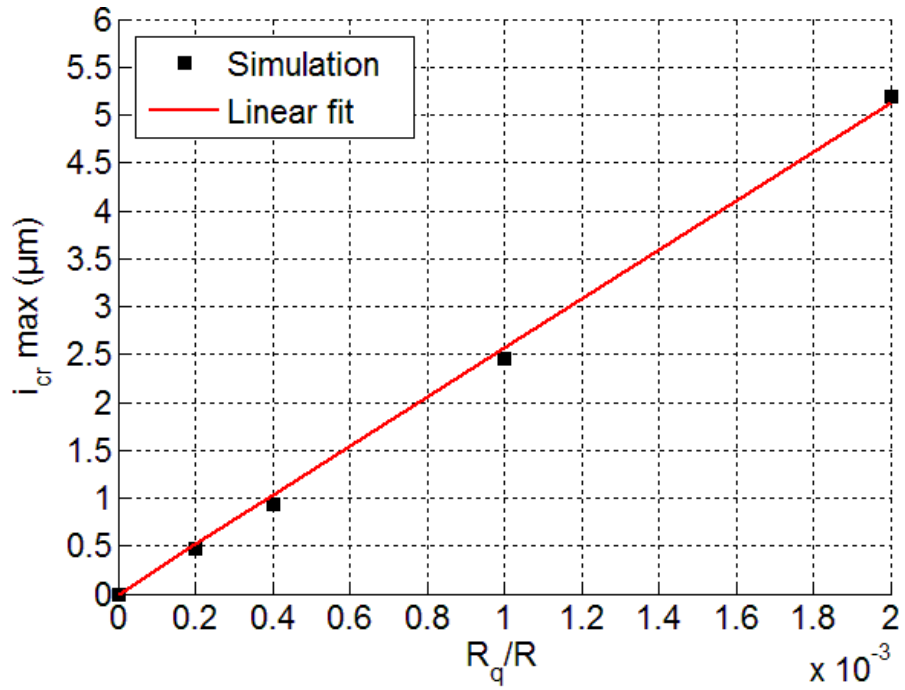
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Figure 11 Critical indentation depth at different normalised roughness values

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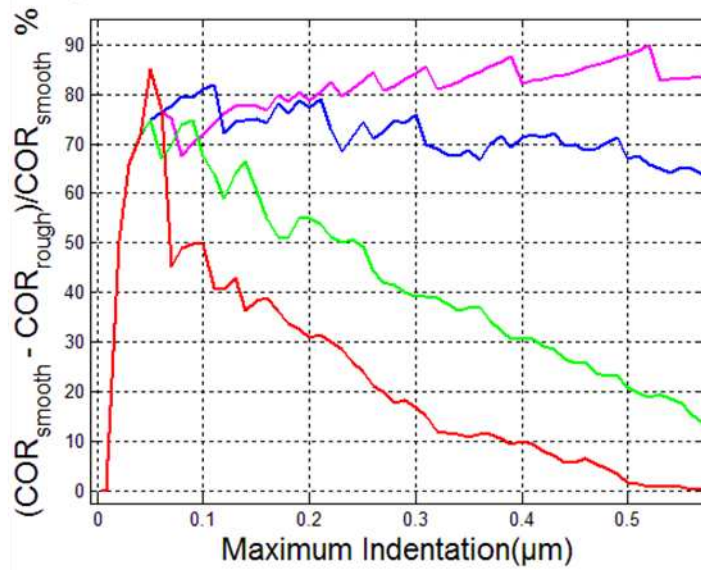
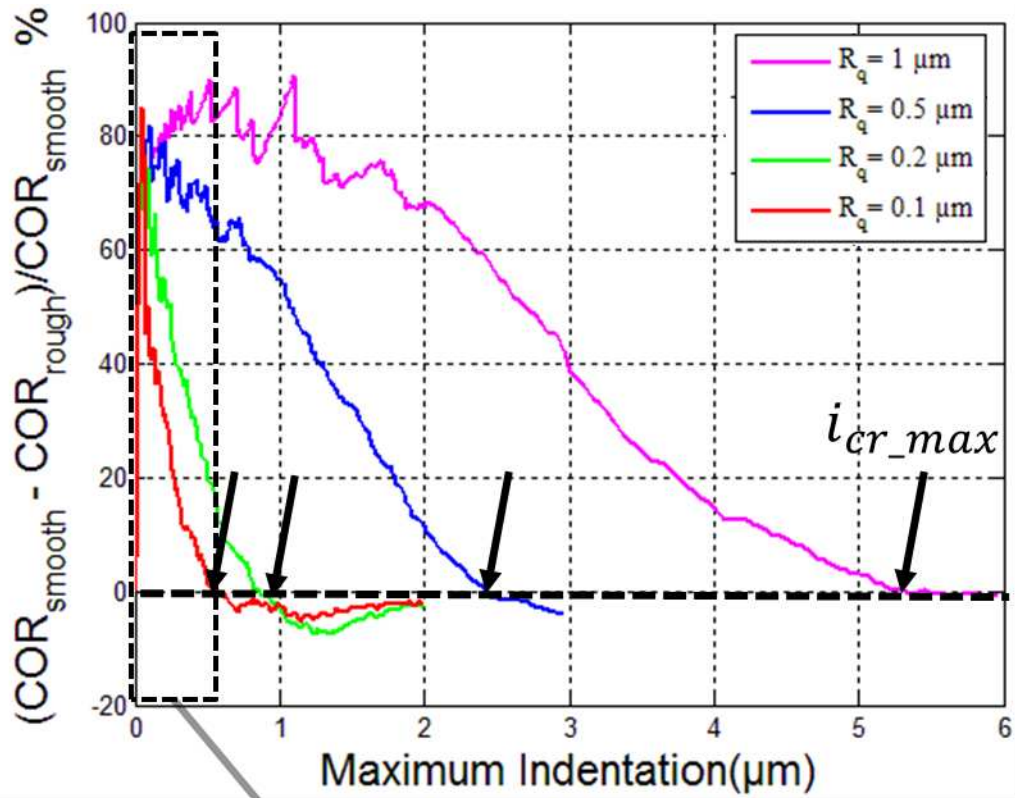
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Figure 12 The difference in COR for rough and smooth surfaces.

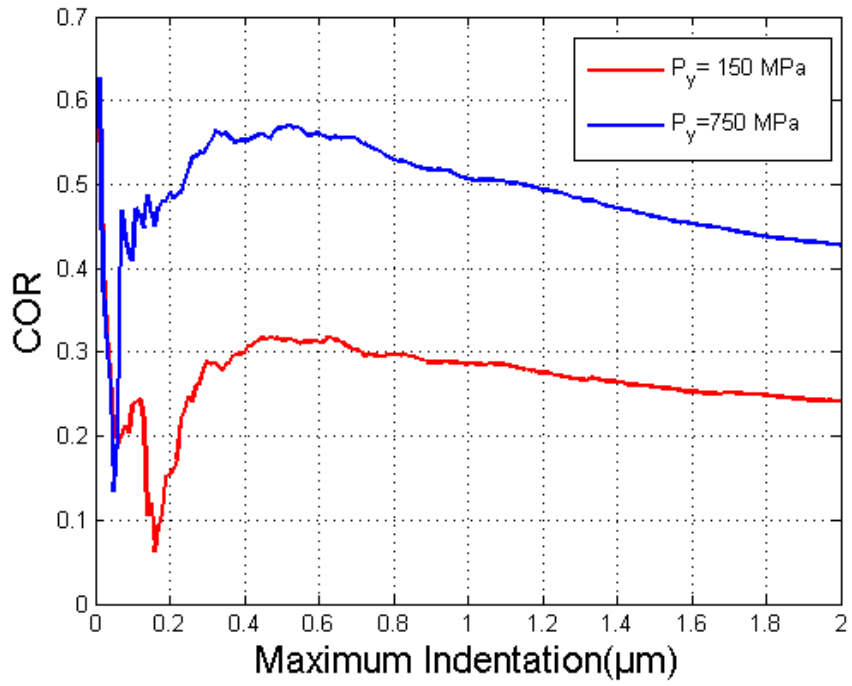
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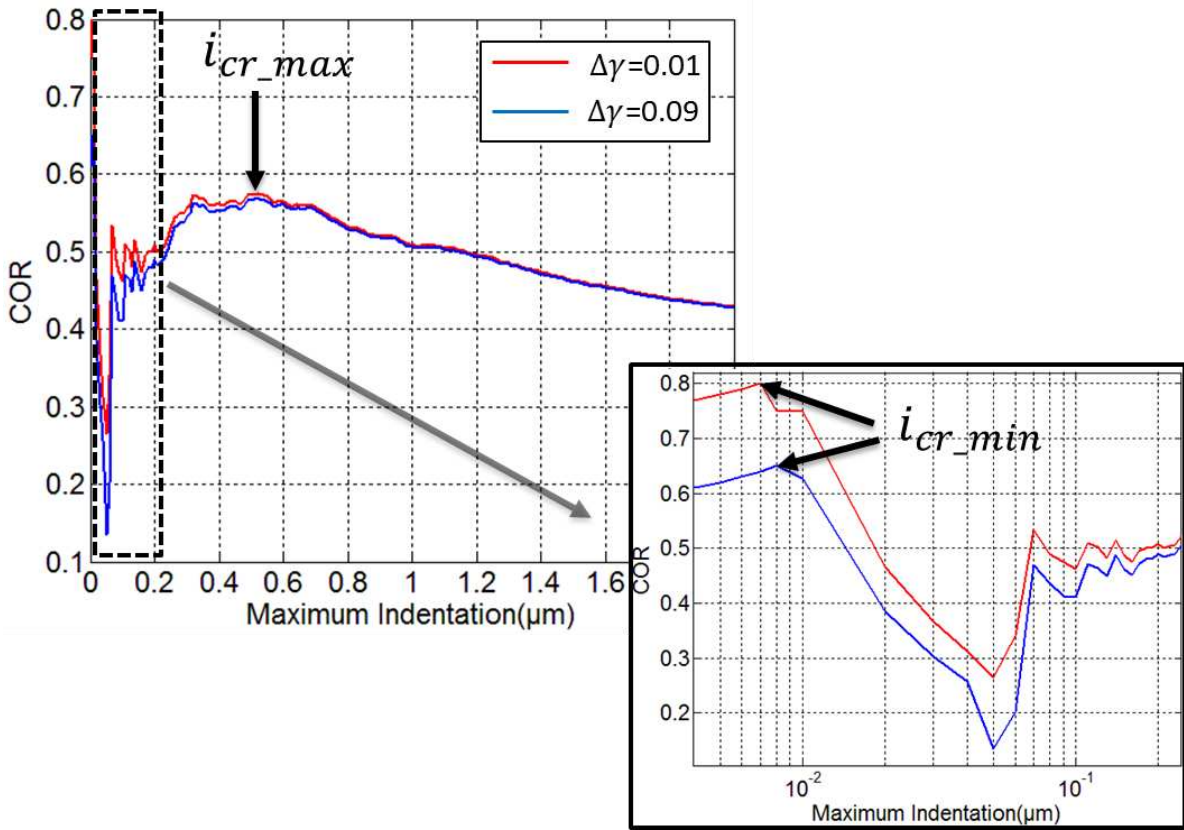
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Figure 13 Effect of yield stress on the COR for rough surface with R_q= 0.1 μm

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Figure 14 Effect of surface energy on the COR for rough surface with $R_q=0.1\mu\text{m}$, $E=210$ GPa and yield stress of 750 MPa