Paper No. ICAT371
2nd International Conference on Advanced Tribology, 3-5 December 2008, Singapore

CONTINUUM ANALYSIS OF ATOMISTIC CONTACTS

Simon Medina[1] and Daniele Dini[1,*]

[1]Department of Mechanical Engineering, Imperial College London
*Corresponding author (E-mail: d.dini@imperial.ac.uk)

KEY WORDS: Continuum Mechanics, Rough Contacts, Atomistic Simulations,

ABSTRACT

We have recently applied a multilevel multi-integration technique to numerically solve the normal and tangential loading of rough surfaces in Hertz-type contact problems [1]. After the qualitative analysis presented in [2], a more refined attempt to generalise the results obtained using continuum mechanics-based approaches and to extend their validity to nanoscale contacts is performed here. The results of the continuum simulations are compared to those reported in the literature at atomic level [3, 4]. It is shown that the use of the rough contact idealisation described here is capable of partially reconciling continuum mechanics and atomistic simulations by capturing some of the features that cannot be captured by the means of conventional Hertzian theory. The potential insight gained using atomistic simulations and the limitations of continuum mechanics in describing some of the physics governing the interactions between rubbing bodies are also discussed.

INTRODUCTION

The use of continuum mechanics for the analysis of contacts is often a most acceptable and convenient approach. With the increasingly common and important cases of atomistic scale contacts, however, the limitations (and potential errors) of its fundamental assumptions have become highlighted. As the scale of analysis approaches atomic level, the characterisation of the substrate as a continuum becomes less and less credible. Molecular dynamics simulations may then appear to be a more appropriate method for modelling contacts on this scale, but is not without downsides, not least of which is the computational time required.

A large proportion of the errors associated with continuum mechanics can come from the specification of the continuum surface. Often the surfaces are assumed to be smooth on a macro scale; this is an unnecessary simplification and a more accurate representation of the surfaces will extend the validity of the continuum approach. With fast solution techniques, continuum mechanics may then still be the more suitable method for analysis of nanoscale contacts. Here, we assess the use of continuum mechanics at the lowest feasible limit of atomic scale contacts.

Recently, Luan and Robbins have modelled the contact of a spherical tip, of the size found in atomic force microscopes, on a flat substrate using atomistic simulations based upon Lennard-Jones potentials [4]. They demonstrated the significant errors that are produced by the usual smooth continuum analysis. Different crystal lattice arrangements for the tips were analysed, for which varying contact responses were observed. They suggested that each tip form was identical on the continuum scale. In particular, although recognising that the local surface roughness at atomic scale could play a very important role in reconciling continuum and atomistic simulations, they asserted that one of the main difficulties in applying continuum theory to atomistic contacts is that it not capable of representing nanoscale asperities. This is due to the fact that it seems not possible to uniquely define the root mean squared (rms) roughness of such surfaces. Luan and Robbins, however, did not consider the possibility of analysing the contacts under investigation as "real" rough surfaces instead of relying on classical representation of rough surfaces in contact based on the use of such parameter.

This is indeed possible and here we show how to differentiate each such tip on a continuum scale by representing the continuum boundary as a rough surface formed by the contours of the atomic lattice. Each atom is considered as a sphere of diameter σ, where σ corresponds to the atomic diameter of the Lennards-Jones solid. Although the notion of varying pressures over an atomic diameter is clearly inaccurate, the representation of the surface features at the sub-nanometer scale may be sufficient to allow analysis of AFM tips and similarly sized contacts.

The contact is solved using the Multilevel Multi-integration technique of Venner and Lubrecht [5] which we recently applied to the analysis of multiple asperity and rough macroscale contacts [1].

RESULTS & DISCUSSION

Results were obtained for the contact between a flat substrate and various forms of tip, each with mean diameter 100σ. The flat substrate was representative of an FCC crystal with [001] surface. Five different tip forms were analysed, similar to those investigated in [4]. A bent commensurate tip was formed by maintaining the lattice form of the substrate but displacing the atoms to generate the required radius. A bent incommensurate tip was formed identically, but with σ and thus atomic spacing of 0.99437 times that of the substrate (leading to non-aligned atoms). A stepped cut tip was formed by removing atoms that fell outside of the required tip radius; an amorphous tip was formed likewise, but from an amorphous arrangement of atoms.

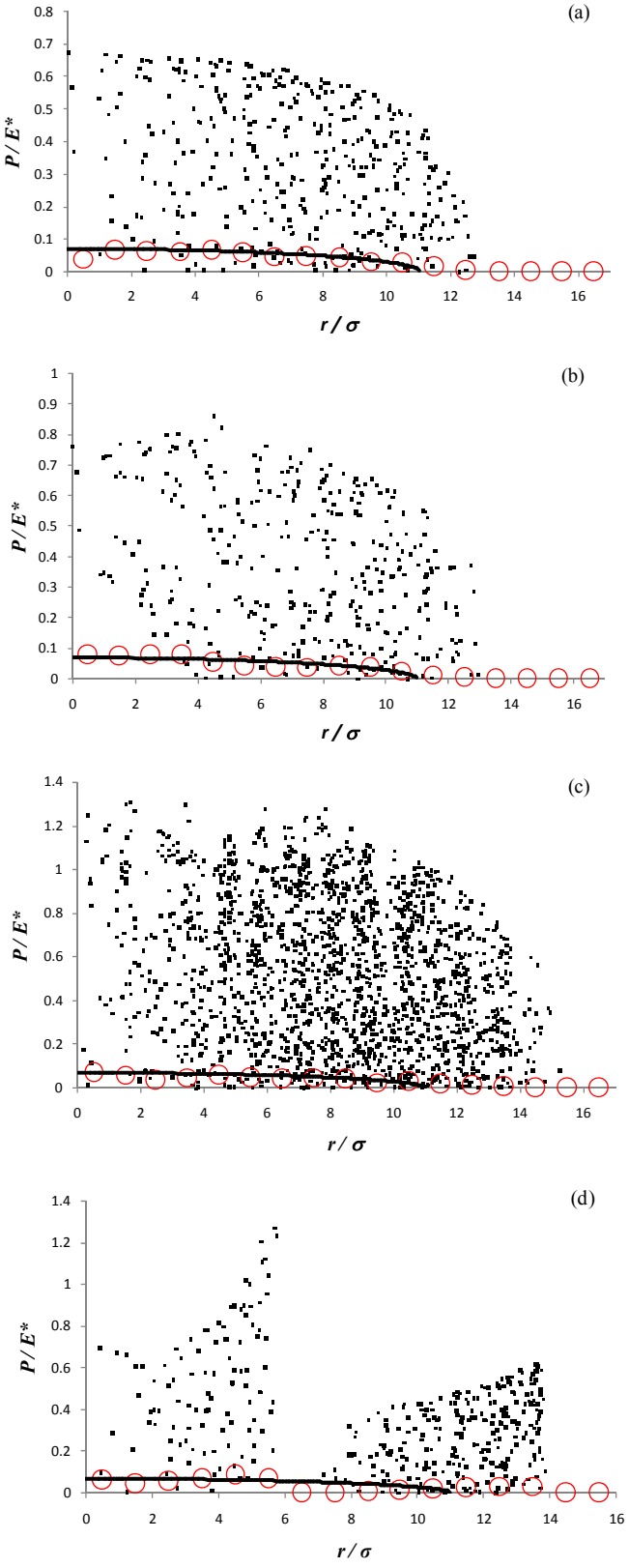

Figure 1: Local pressure vs. radius for each tip: (a) bent commensurate, (b) bent incommensurate, (c) amorphous (d) stepped. The points indicate pressures of each node that is in contact; circles indicate the average pressure over an annulus of width σ, centred on the indicated radius (including non-contacting nodes). The smooth contact Hertz solution is shown as a solid line.

Finally, a smooth tip was possible in this analysis, which could not be directly modelled by atomistic simulations; here a smooth tip on smooth substrate analysis was performed which is directly comparable to the theoretical Hertz analysis. The reasoning behind differences for each tip form is discussed in [4] and is not repeated here. Instead we focus on comparisons between results for the atomistic and continuum approaches.

Figure 1 shows the variation of pressures with radius from tip centre. In [4], the pressures were taken as the atomic force divided by the atomic area; here, the pressures are available over any scale down to the discretisation size (256 x 256 nodes). A node-by-node plot of pressures thus shows a much greater spread of values at constant radius than the analogous atomic representation reported in [4]. It should be noted here that the black dots in Figure 1 indicate nodal pressures; nodes which were not in contact (the majority) are not shown. Averaging the pressures over a region of size σ^2 gives a closer approximation to the atomic model. The red circles in Figure 1 give the average pressures in radial bins of width σ, which can be compared better with the atomistic analyses. The differences observed by Luan and Robbins are also visible with this continuum analysis.

The variation of normal approach, δ, and contact radius, a, with applied load are shown in Figure 2(a) and (b). As in [4], the normal displacement shows the smallest deviation from Hertz, whilst the contact radius is generally larger than the Hertz prediction, with the largest discrepancies obtained for amorphous and stepped tips.

The most significant advantage of using atomistic simulations may be the ability to examine tangential loading directly. With our continuum analysis, tangential loads can only be examined *after* specifying an appropriate friction coefficient, f. Amonton's friction law is assumed here to apply locally, such that the nodal tangential force, $q \leq fp$. The tangential displacement can then be calculated using continuum mechanics, assuming a semi-infinite half space (as done for the normal contact solution). To obtain the lateral stiffness, the displacement at a remote point in the body is obtained for a given applied load. For the tangential stiffness results below, a friction coefficient of 0.63 was assigned, as found by the simulation of Luan and Robbins for two of the tips under consideration, and the limiting frictional load was applied (fN). The tangential stiffness of the various tip forms are shown in Figure 2(c). Some of these values differ significantly from those in [4], and are much closer to the Hertzian solution than found by Luan and Robbins. The semi-infinite half-space is a poor approximation when the scale of the roughness is comparable to the tangential displacements. Combined with this, the continuum analysis assumes interfacial stick; the atomistic simulations included the interfacial compliance, which greatly reduced the stiffness from that of the smooth continuum model.

The lack of frictional predictions is not necessarily due to the fundamental continuum assumption of a continuous material, but it is difficult to incorporate local frictional characteristics within a continuum analysis. Additionally, without the limiting assumption of a half-space for determining tangential displacements, a

continuum analysis is unlikely to offer a computational benefit over atomistic simulations.

Despite these shortcomings, an important advantage of the continuum analysis is that it can be scaled to larger sized contacts (still maintaining atomic scale features) with a lower computational penalty than atomistic simulations. Besides the relatively higher two dimensional penalty, a suitable molecular model would also require an increasing substrate depth, not applicable to continuum models, compounding the problem of solution time.

Luan *et al.* [6] have recently attempted to improve the scalability of atomistic solutions by coupling a finite element solution for large scale features to an atomistic model. The present results suggest that a continuum analysis (for medium to large scale features) coupled to atomistic simulations to account for frictional effects and small scale features may be used, thus narrowing the gap between the use of continuum and atomistic simulations for the study of rough contacts at the nanoscale.

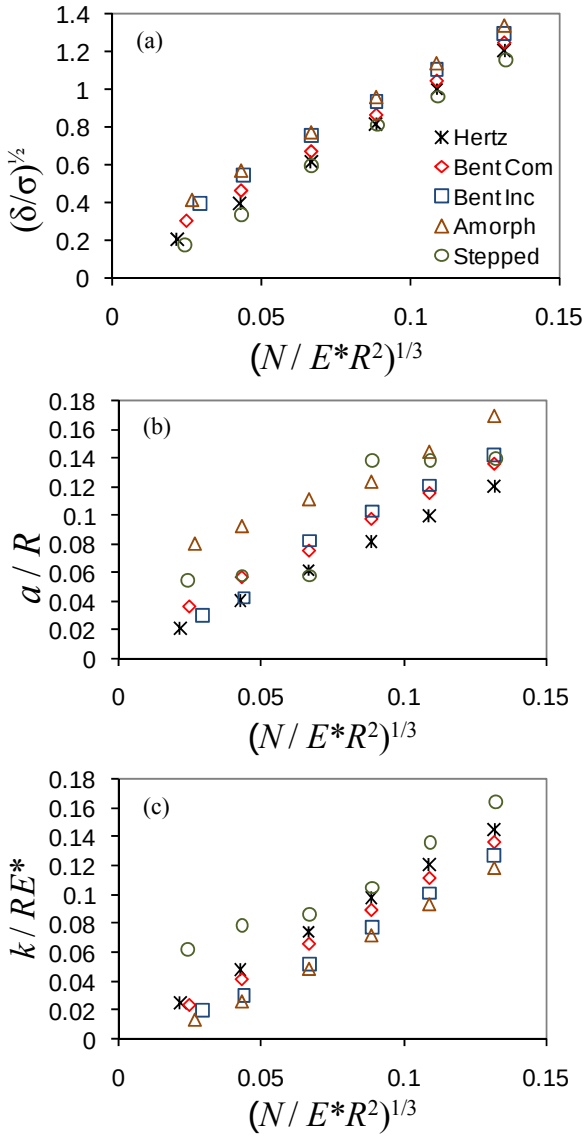

Figure 2: Effect of normal load on (a) normal displacement, (b) maximum contact radius, and (c) tangential stiffness. Plots are dimensionless and expressed as powers such that the Hertz solution is a straight line, and are thus comparable with [4].

CONCLUSIONS

A continuum mechanics analysis of an atomistic scale contact has shown results not only qualitatively but also quantitatively comparable to those obtained by the means of atomistic simulations. Different atomic arrangements, with same mean tip radius, show different pressure distributions, contact stiffness and area corresponding to the results obtained by Luan and Robbins [3, 4] considering the local atomic interactions between rounded tips and substrates. To our knowledge, it is the first time that continuum mechanics has been used to describe the physics of contacting bodies at the atomic level.

A limitation of the current analysis method is that the frictional force cannot be predicted. Whenever in the presence of tangential interactions, one must make assumptions about how frictional forces depend on contact area and loads. At atomic length scales methods such as molecular dynamics and atomistic simulations or quantum mechanical methods must be employed which take into account the atomistic and chemical nature of real surfaces in order to shed light on the very local nature of the frictional behaviour. However, once that information is available, and, for example, a constant friction coefficient is assumed between the contacting bodies, lateral compliance can be assessed quickly.

The speed and simplicity of a continuum model may be advantageous whilst still revealing important behaviour associated with atomic level features. In this respect, the present contribution constitutes a fundamental step in understanding if atomistic resolution can be achieved by stretching the boundaries of applicability of continuum contact mechanics.

REFERENCES

[1] Medina, S., Dini, D., Olver, A.V., and Hills, D.A., Fast computation of frictional energy dissipation in rough contacts under partial slip. *ASME/STLE Joint Tribology Conference*, Miami, 20-22 October 2008.

[2] Dini, D., Between continuum and atomistic contact mechanics: could we bridge the gap?. *ASME/STLE Joint Tribology Conference*, San Diego, 22-24 October 2007.

[3] Luan, B. Q. and Robbins, M. O., The breakdown of continuum models for mechanical contacts. *Nature* 2005, Vol. 435 (7044), pp. 929-932.

[4] Luan, B. Q. and Robbins, M. O., Contact of single asperities with varying adhesion: Comparing continuum mechanics to atomistic simulations. *Physical Review E*, 2006, Vol. 74, 026111.

[5] Venner, C.H. and Lubrecht, A.A., *Multilevel methods in lubrication*, 2000, Elsevier.

[6] Luan, B. Q., Hyun, S. Molinari, J.F., Bernstein, N. and Robbins, M.O., Multiscale modeling of two-dimensional contacts, *Physical Review E*, 2006, Vol. 74, 046710.