

**Properties of a Single Asperity and the Interface Between Molecular Dynamics and  
Continuum Mechanics: A Commentary\***

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**I. Introduction**

The speakers in this session attempted to bridge the large spatial gap between the atomistic processes occurring at a sliding interface and the continuum description of such processes. This task is indeed formidable. One may ask why should we study such elementary processes at all if what we are really interested in is a global picture of friction. Real surfaces are uneven, impure, and may be covered by nasty things like lubricants specifically placed there to modify frictional behavior. Isn't the real world of friction too "dirty" to be studied by surface science techniques? Indeed, even if we were to understand the interaction of every geometry of single asperity under every environment, how to average this information to produce a model of friction is unknown. Does this mean that we shouldn't attempt to measure and calculate these simple processes? I think not. Understanding the response of a single asperity is an important essential element which will lead to a thorough predictive understanding of friction. But clearly our work cannot end with the study of single asperities. There are two critical phenomena which have to be added to a single asperity model: first the inclusion of a distribution in both size and location of single asperities and second the role of microstructure evolution. Clearly single asperities do not respond independently from each other. The proximity of two asperities changes both the local stress distribution as well as the contact area. I believe the greatest challenge that faces us is how to assemble the vast amount of single asperity data that we can generate and from it create useful engineering models.

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## II. The Session

The session began with a talk by N. Agrait on experimental techniques to measure the mechanical properties of a single nano-asperity. These techniques are in their infancy. It is exciting to realize that we are now in the position of being able to measure mechanical properties of such a small volume of material. Using a combination of scanning force and tunneling microscopy the force necessary to deform a small volume of material is measured. The experiment measures the deformation of ~20 nm wide necks between a probe tip and the substrate. Quantized transitions, presumably in neck geometry, occur at critical stresses. Using approximate contact areas the critical stress is found to be 2-6 GPa in gold. These stresses are significantly higher than the yield strength of bulk gold, leading Agrait to conclude that deformation occurs by nondislocation mechanisms similar to those presented by U. Landman from molecular dynamics simulations later in the session.

Landman presented the results of numerous molecular dynamics calculations using empirical and semi-empirical atomic potentials. His results using an embedded atom method potential for gold showed the stepped behavior that Agrait discussed above. The size of the calculated asperity was about an order of magnitude smaller than that measured by Agrait. Landman also presented results of molecular dynamics simulations of two asperities sliding by each other with an alkane between. The alkane was modeled using simple three-body potentials developed to simulate near equilibrium behavior. The alkane metal interaction was an empirical two-body potential fit to desorption energetics. The simulations showed molecular layering of the alkanes induced by the approach of the asperities. The layering produced oscillations of the friction force.

R. Phillips presented a novel method for including atomistic information in a continuum finite element boundary value problem in a seamless fashion. The method involves replacing the traditional elastic or elasto-plastic constitutive law with a simple atomistic calculation that embodies the local atomic arrangement. Phillips demonstrated that

the method reproduces the results of a purely atomistic calculation of dislocation core structure of Al modeled with an embedded atom method potential. He then applied the method to indentation of Al with a rigid indenter. Both a punch (2.3 nm) and wedge (66 nm) geometry were used. Quasi-static indentation was performed to a depth of 0.6 nm. In the case of the punch indenter multiple dislocations were emitted at the edge of the punch, while for the larger wedge no dislocations were emitted.

The final talk of the session was by K. Johnson who discussed continuum modeling of both adhesion and friction and their relationships. Adhesion was considered as a mode I fracture process of a sphere in contact with a plane. The primary result is that this analysis yields an adhesion map showing rigid, elastic, and plastic behavior of adhesion as a function of two materials parameters. Friction was modeled using an elastic sphere interacting with a plane under mixed mode loading. This analysis results in a relationship involving the properties of the interface which are not known from continuum theory. This relationship attempts to quantify the mixed mode loading effect.

### **III. Critical Comments**

The experiments by Agraït are very encouraging in that it appears that we are now at the point of being able to measure mechanical properties of extremely small volumes of material. It must be realized that these new techniques have been applied to only very idealized systems. To be useful for friction modeling these experiments must become quantitative. One weakness noted is that the area of interaction is not well known. In general a quantitative knowledge of the geometry of the asperity being measured is necessary if these measurements are to be compared to atomistic calculations. Impurities must be added at the interface to assess their important effect. Mixed mode loading must be imposed.

The molecular dynamics calculations of Landman are excellent for looking at the underlying physical mechanisms of friction. To use these computations as a basis for a global friction model they must be improved significantly in a number of ways. The boundary conditions used in the calculation of two interacting asperities are very restrictive. The rigid model used does not allow plastic or even reasonable elastic response of the material near the asperities. Thus the asperity response is not realistic and any response of the alkanes is questionable. Another question is the interatomic potentials. For the case of metals the embedded atom method is probably sufficient to capture the material response. In the case of lubricants, however, the simple equilibrium potentials cannot capture any chemical effects which are likely to be important in friction processes. Better potentials are needed to investigate chemistry and also the metal (oxide)-organic interactions. Finally molecular dynamics suffers from an inherent time scale problem. Since all of the atomic vibrations are followed, only mechanisms with time scales in the nanosecond range are easily examined. The extrapolation of these process to longer times is usually difficult.

The method developed by Phillips is an excellent first step in solving the boundary condition problem mentioned above. Computations using this method have the potential to develop atomistically based plasticity models. To be useful in friction modeling the method must be extended in at least the three following areas. The formulation of the model now is in terms of a single element. Impurities must be added. This task appears to be a difficult one in the current context of the model. Second, time (dynamics) must be included. Because of the seamless fashion of this model it appears that adding dynamics will be possible in contrast to earlier finite element/atomistic models where the discrete atomistic region was embedded in a finite element mesh. Third, three dimensional capability must be added. The problem here appears to be the implementation of robust 3-D remeshing algorithms. The time scale limitation discussed above also is a limitation in these calculations.

The continuum modeling of adhesion discussed by Johnson appears to be in reasonably good shape. It is not useful, however, if material properties are not known. The extension to friction is weak even in the case of pure elastic behavior. Plasticity has not been included in the friction modeling. Again the continuum models need to have interfacial properties which in general are not known. The formulation of the continuum model does not contain an interfacial region with properties different from that of the sphere or contact plane. This region exists and its time dependent properties should be included in the models.

#### **IV. Future Directions**

The path to development of a predictive global friction model based on microscopic mechanisms seems clear but extremely difficult. The response of a single asperity must be quantified using both experiment and simulation. By response here I mean the transient deformation and the associated stresses and strains produced by external loading. Unfortunately there are an inordinate number of variables to consider including asperity geometry and composition, environment (lubricants, impurities, etc.), and loading conditions. It is important that the characterization does not get mired in a sea of technical details not important to the ultimate predictive model. This data needs to be incorporated into continuum models of a single asperity such as those presented by Jackson. These models will have to be extended and reformulated to be consistent with the single asperity data base. To be useful these models should be based on the microscopic mechanisms determined through the above experiments and simulations and not on phenomenology. Finally a global model needs to be developed that includes the interaction of a distribution of single asperities each of which are described by the single asperity continuum model. This model need to include the role of microstructure evolution.

We consider the above path in a bit more detail. On the experimental front what is necessary is measurement of the mechanical response of an asperity with known geometry to mixed mode loading conditions. Inclusion of environmental effects (lubricants or impurities) is important. The idea here is to create a data base so that a generic response model of a single asperity can be generated. The experiments will act as a critical proving ground for the reliability of atomistic calculations which can be performed more easily than experiment. In addition the simulations can be controlled much more easily than experiment and thus are easier to use as a data base for continuum models. These calculations need to include realistic potentials. However, the detail of the potentials must be limited so that it is computationally feasible to handle the number of atoms that is necessary to accurately represent the real boundary conditions. Potentials for metals must be able to reproduce the elastic and plastic bulk behavior and bond breaking and formation at free surfaces. The potentials for lubricants must reproduce the fluid behavior of the lubricant as well as the chemistry that occurs under extreme loading. Realistic boundary conditions must be employed that represent actual far-field loading conditions and do not affect the local friction mechanisms. Both the simulations and experiments would elucidate the friction mechanisms to be included in the single asperity continuum models.

One of the crucial missing links appears to be a model that combines the properties of a distribution of asperities into a global friction model. Development of such a model would enable both experimentalists and theorists to understand the sensitivity of the macroscopic friction to the details of single asperity properties. Such knowledge would simplify their task of characterization of the single asperity. Development of this model appears to be the most challenging task. Interaction of sliding surfaces causes asperities to change their geometry, break off from the surface to mix with the lubricant, or even worse, lose their identity by mixing with bulk material, changing the near surface microstructure and hence bulk mechanical properties. All of these phenomena must be included in the global model. Clearly this is a challenging task!