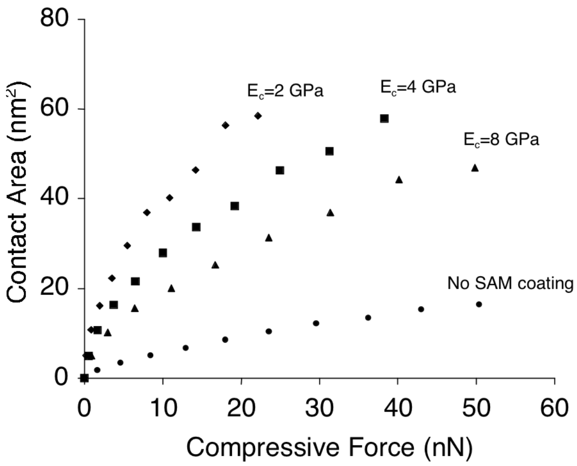

Figure 2. Calculated contact area as a function of the SAM's Young's modulus for a 27-nm radius of curvature silicon tip indenting a 2-nm thick SAM coating on a silicon substrate (ν_c = 0.4).

analytic solutions might be applicable if the relatively compliant, but thin, SAM coating can be ignored. For this reason, a series of preliminary calculations were performed to evaluate the effect of a SAM coating. These calculations ignored adhesion and used the geometric model shown in Fig. 1. The polysilicon was treated as a linear elastic material with a Young's modulus, E, of 161 GPa and a Poisson's ratio, ν, of 0.23. The OTS-SAM coating was assumed to be an isotropic, linear-elastic material (undoubtedly an oversimplification), and a range of polymer-like Young's moduli, E_c, were considered (coating Poisson's ratio, ν_c, was fixed at 0.4). Also note that in the simulations the tip was pushed at a sufficiently slow velocity (~ 1 m/s) to produce a quasi-static response. Figure 2 indicates that the SAM coating has a significant effect on contact; it reduces contact pressure and increases contact area. Consequently, any finite element contact analysis must explicitly include the relatively compliant SAM coating.

The effect of adhesion was considered next. The adhesion vs. separation model was based upon a Lennard-Jones potential and corresponds to the adhesive force/unit area between two half-spaces [5]. Results for three adhesion levels are plotted in Fig. 3 for a 2-nm thick SAM coating (E_c = 8 GPa, ν_c = 0.4). Interestingly, even when a relatively compliant coating is present, the results appear to be DMT-like in that the elastic contact stress distribution is the same as that without adhesion, while its integral equals $P+2\pi WR$, where P is the applied load and R is the radius of curvature of the tip [5]. Thus an effective load $P + 2\pi RW$ collapses the Fig. 3 results to a common curve (Fig. 4). This greatly simplifies the required analysis since one does not need to perform separate calculations for each adhesion value of interest; adhesion can be taken into account simply through an effective load.

What is required is a relationship between friction force and effective load in terms of the two free parameters, W and τ^*. Note, however, that friction force is taken to be equal to the product of contact area and τ^*, which is assumed to be a constant for a given pair of surfaces. Consequently, the finite element contact analysis only needs to determine the relationship between contact area and applied load. This must be done for each combination of SAM, tip, and substrate material properties (e.g., various E_c) and geometric parameters (e.g., R and SAM layer thickness, h_c) of interest. For the range of applied loads relevant to our AFM friction tests, the contact area vs. applied load relationship can be fit quite well by a simple power-law relation. Using this fact, and based upon di-

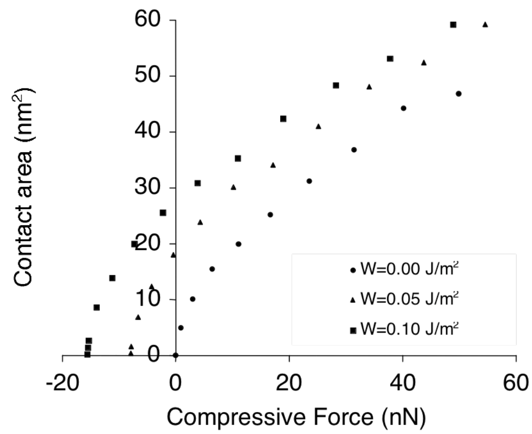

Figure 3. Calculated contact area as a function of the work of adhesion, W, for a 27-nm radius of curvature silicon tip indenting a 2-nm thick SAM-coated silicon substrate (E_c = 8 GPa, ν_c = 0.4).

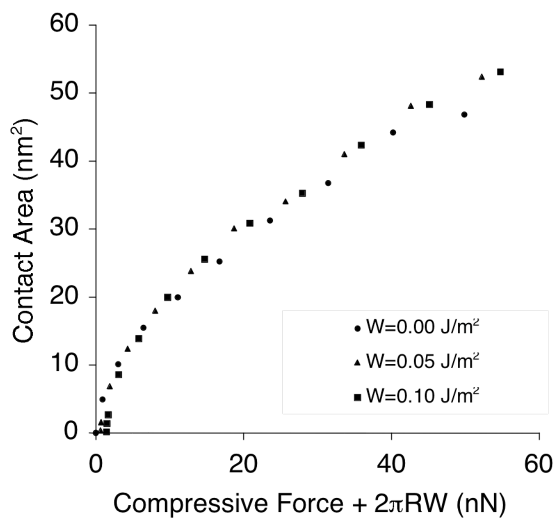

Figure 4. Calculated contact area as a function of the DMT-like effective load for a 27-nm radius of curvature silicon tip indenting a 2-nm thick SAM coating on a silicon substrate (E_c = 8 GPa, ν_c = 0.4).

mensionality arguments, the following relationship was determined:

$$\text{Friction Force} = \tau^* \pi \left(\frac{3PR\left(1+\frac{\bar{E}}{\bar{E}_c}\right)}{4\bar{E}} \right)^{2/3} A\left(\frac{P}{\bar{E}_c h_c^2}\right)^b \qquad (1)$$

where $\bar{E} = E/(1-\nu^2)$ and $\bar{E}_c = E_c/(1-\nu_c{}^2)$. The parameters A and b have been determined from a series of finite element calculations, and depend on elastic and geometric properties. Table 1 lists current estimated values for these parameters. Note that these parameters are thought to be applicable when h_c/R values between 0.057 and 0.074, for $P/\bar{E}_c h_c^2$ values between 0.02 and about 2, and for $\nu = 0.23$ and $\nu_c = 0.4$.

Table 1. Parameters used in Friction Force vs. Applied Load relationship (Eq. 1)

$\bar{E}_c/\bar{E}$	A	b
0.014	0.65	-0.11
0.028	0.66	-0.11
0.056	0.66	-0.09
0.112	0.73	-0.08

Figure 5 demonstrates the use of the Friction Force vs. Applied Load relationship (Eq. 1) to determine the τ^* and W values corresponding to two different sets of AFM friction measurements. As an aside, the plotted experimental results are for two nominally identical tests, indicating current issues with day-to-day variability in AFM-friction measurements that are believed to be due to contamination of the tip. The analytic relation closely matches the experimental data for the indicated τ^* and W values. These fits assume E_c = 8 GPa. It must be emphasized that the fits assume that the values of R, h_c, E, ν, E_c, and ν_c are independently known. There are any number of equally good fits when the ratio $\tau^*/E_c^{2/3+b}$ is held fixed (follows from Eq. 1 and the fact that A and b are a weak function of E/E_c for the range of values considered, Table 1). This presents some difficulty since E_c, and ν_c are difficult to measure. There are some potential approaches for experimentally determining E_c, but these are difficult measurements [3]. One may also be able to make estimates of SAM properties from the results of molecular dynamic simulations of SAMs [6, 7].

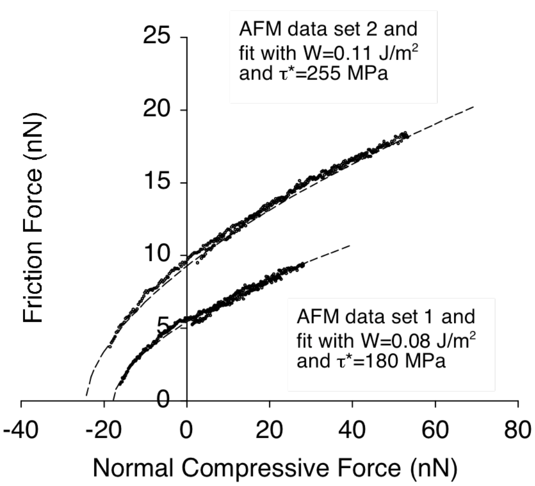

Figure 5. Values of work of adhesion, W, and shear junction strength, τ^*, parameters in the analytic relationship for Friction vs. Normal Force that produce a good fit to AFM friction test data (E_c = 8 GPa, ν_c = 0.4).

Acknowledgements

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04 94AL85000.

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