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Atomistic mechanisms of adhesion and hysteresis during contact

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ABSTRACT

The use of Atomic Force Microscopes to measure mechanical properties of soft samples beneath it has been hindered by a lack of understanding of the mechanisms responsible for the observed depth-dependent hysteresis in the load (P) vs. indentation (h) measurements. This phenomenon is not captured by classical contact theories, such as Hertz, JKR and Maugis-Dugdale. Inelastic effects like plasticity or viscoelasticity were generally held responsible for this phenomenon. However some experimental results [1,2] strongly hint at the possibility of having depth-dependent hysteresis during perfect elastic contact.

Atomistic simulations using empirical potential models were performed to test whether we could find depth-dependent hysteresis during perfect elastic contact, as well as to gain understanding into the plausible mechanisms operating behind this phenomenon. The simulations consisted of calculating the net interaction forces between two bodies as they were quasistatically brought into and out of contact at T=0 K. The elastic deformation and surface energies were also computed during the contact process. The simulations were performed for different levels of adhesion between the bodies. It was seen from the simulations that repeatable depth-dependent hysteresis can indeed appear without plasticity. Additionally, the contact region grew/receded through a series of discrete jumps. This discrete nature of contact growth/recession is seen to contribute to hysteresis.

These simulations results will be presented along with an analytical model that shows how microscale roughness may manifest itself as the appearance of hysteresis in the measured P-h curve. This model also predicts depth-dependent hysteresis during elastic contact. The predicted P-h curves may be used to obtain unique estimates for elastic mechanical properties in probing experiments of soft materials where similar hysteretic mechanisms may be operating.

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