Particle adhesion at the nano-scale

K Kendall[1]*, C W Yong[2] and W Smith[2]
[1]*Chemical Engineering, University of Birmingham Edgbaston B15 2TT*
[2]*CCLRC, Daresbury Laboratory, Warrington WA4 4AD*

*k.kendall@bham.ac.uk

This paper attempts to connect macroscopic observations of particle adhesion with the known interatomic forces which bind particulate interfaces together, by studying contact between a plane surface and a sphere of smaller and smaller diameter. The fracture of a contact between a plane and a macroscopic sphere depends on the non-uniform stress distribution across the contact spot, causing atomic attraction at the edges of the contact region. Interface atoms some distance inside the contact region do not contribute to the adhesion. In fact, these inner atoms are in compression and are pushing the particles apart rather than causing adhesion. When a smaller sphere adheres to a plane at the nano-scale, this non-uniform stress distribution cannot be possible and the stress across the contact must be more even. To prove this hypothesis, sodium chloride crystal nanoparticles have been considered. The atomic interaction potentials have been used in a molecular dynamics model to calculate the adhesion forces and contact stress distributions during particle pull-off as sodium chloride particles are altered in size. The results show that there is a stress concentration at the contact edge even for the smallest particles with 16 atoms in contact.

Keywords: particle adhesion, molecular dynamics model, fracture mechanics, nanoparticles