INCORPORATING SHORT-RANGED REPULSIVE FORCES TO IMPROVE HAMAKER CONSTANT ESTIMATES OF SOLID SYSTEMS

Understanding particle adhesion is crucial to the optimal performance of various processes ranging from the manufacturing of pharmaceuticals, consumer goods and semiconductors to the design of explosive detection systems. The van der Waals (vdW) forces between atoms and/or molecules are of particular interest as they are always present in all systems and often times are the dominant adhesive force between neutrally charged materials. The vdW forces acting between two discrete materials through a given medium are quantified by the Hamaker constant, A. There are many different instruments that have been used to estimate Hamaker constants such as the atomic force microscope (AFM), surface force apparatus, centrifuges and optical goniometers. The AFM proves particularly useful for this as it can measure interaction forces from piconewtons to micronewtons for a wide range of solid particle-substrate systems; moreover, it can characterize the substrate's topography to the nanometer scale. The expansion of a model of the vdW forces to improve existing methods for estimating the Hamaker constant of solid systems is the focus of this work.

An AFM can characterize the interaction force between two solids through deflection-distance (DD) curves. DD curves are collected by bringing an AFM probe into and out of contact from a substrate of interest. DD curves tend to have two discontinuities known as the approach to contact (AtC) deflection or d_c and the pull-off deflection or d_{PO}. Existing AFM approaches solely focus on one of the two. What both kind of approaches have in common is that in most cases only attractive forces are considered, leaving repulsive forces to be neglected or only implicitly acknowledged. AtC methods generally neglect repulsion as it is not needed to predict the limit of stability that gives rise to d_c. Some pull-off methods acknowledge repulsion through contact-mechanics, i.e. using JKR model, while the majority of approaches implicitly account for repulsive forces through the use of a fixed minimum separation distance. Although the minimum separation distance is meant to represent the smallest gap between atoms on the AFM probe and the substrate, it is often invoked with minimal justification and used as a mathematical tool to avoid the attractive force from diverging to infinity at contact. Moreover, the majority of existing analytical models only predict a single value of d_c or d_{PO} which is not the case in experiments given that surface roughness (both in the probe and substrate) gives rise to distributions of deflections. Hence there is a need for the development of a model that explicitly acknowledges steric repulsive interactions which can consistently predict d_c- and d_{PO}-distributions based on atom-atom interactions.