Molecular dynamics study of the contact strengths between clean metallic surfaces with nanoscale asperities

HOJIN KIM, ALEJANDRO STRACHAN, School of Materials Engineering, Purdue University, West Lafayette, Indiana, USA — A fundamental understanding of the mechanical behavior of contacting surfaces with nanoscale asperities including their adhesion and friction is critical for MEMS and other applications. We characterize the tensile strength of contacts formed between various clean Pt surfaces such as commensurate contacts between (001) and (111) surfaces and incommensurate (001) ones by using MD simulations over wide range of asperity size. In cyclic closing and opening, the first contact shows significant plastic deformation, leading to a considerable reduction in the contact area. After few cycles, steady state is achieved both contact size and the pullout force. The strength of bridges in both commensurate and incommensurate contacts exhibits strong size effects. Their strength increases with decreasing size until a length of approximately 5 nm below which weakening is observed. Commensurate contacts are stronger than incommensurate ones but only during the initial contacts, after steady state is achieved commensurate and incommensurate (001) surfaces lead to similar strengths.