Molecular dynamic simulation on collision induced cold welding in ceramic nanoparticles

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Cold-welding phenomena in zero dimensional material is investigated by molecular dynamics (MD) in this work. Compared with metal (copper) where cold welding can be introduced by mechanical contact only, ceramic (zirconia) nanoparticles could be cold welded by collision at room temperature, which is a new mechanism that distincts from traditional cold welding. Specifically, two crystalline zirconia nanoparticles are collided with each other in a NVT ensemble. The crystallinity and tensile strength at the bonding region is investigated and discussed. The differences between the outcomes from copper and zirconia are compared. Prediction upon bonding properties between two nanoparticles could provide guidance for nanoscale manipulation and design.

Keywords: cold-welding, molecular dynamic, zirconia, crystallinity