

Molecular Dynamics Study on the Bonding Strength of Direct Diamond Bonding

Speaker:



Dr. Qing Peng
Wuhan University, Wuhan, China

Date: Monday, March 2nd, 2026

Time: 11:00 a.m.

Location: Bldg. 6/Room 125

Abstract:

The performance of next-generation semiconductor devices critically depends on the quality of material interfaces, yet the direct bonding mechanism of diamond -- an ultimate semiconductor material -- remains poorly understood at the atomic scale. Here we present atomic-scale insights into the direct bonding of rough diamond (001) surfaces using molecular dynamics simulations. Our results reveal a characteristic “order–disorder–order” structural evolution at the interface, which facilitates the gradual formation of stable C–C covalent bonds and a significant reduction in system energy. A critical roughness threshold of 0.4 nm is identified, below which the interfacial formation energy increases dramatically by 275%, marking a transition to high-strength bonding. Mechanical pressure is found to be more effective than thermal energy in promoting covalent bond formation across the interface. Furthermore, atomically smooth diamond interfaces can achieve bonding strengths comparable to that of bulk diamond. In this talk, I will also discuss ongoing and future work related to these findings.

Biography:

Dr. Qing Peng is a Professor (Level 3, senior full professor who serves as a discipline leader) in Wuhan University. He received his PhD from University of Connecticut in 2005, MS from State University of New York at Binghamton in 2000, and BS from Peking University in 1998. His research focuses on computational materials physics using multiscale, first-principles, molecular dynamics, and finite-element modeling and simulations. Dr. Peng has published over 300 peer-reviewed journal papers with over 8600 citations and an H-index of 45. Dr. Peng serves as Editorial board member of a few journals including “Scientific Reports”, “Crystals”, “Nanomaterials”. He is on the Worlds’ Top 2% Scientists list. He is also the Chief Scientific Officer of IC Research Technology (Wuhan) CO. LTD.

. All faculty, researchers and students are invited to attend.



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