Hardness of UNCD and Friction of Buried Interfaces

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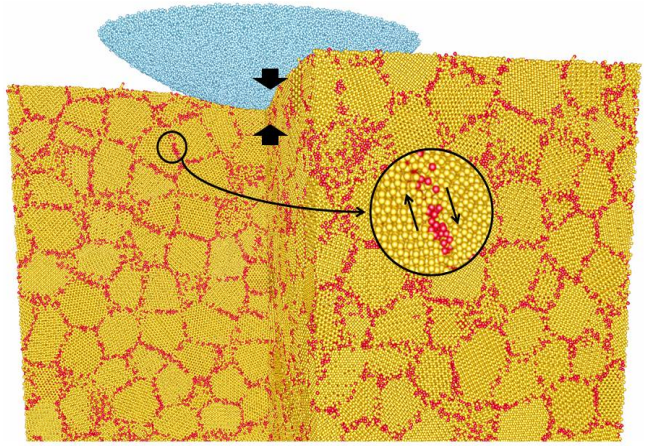
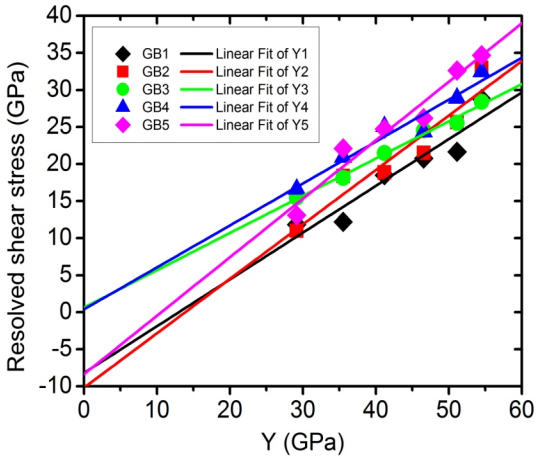
Motivation: Understanding of fundamental mechanisms of friction and wear of ultrananocrystalline diamond (UNCD). Promising material for coating drill bits for oil recovery.
Approach: Massively parallel molecular dynamics simulations of nanoindentation and uniaxial compression.

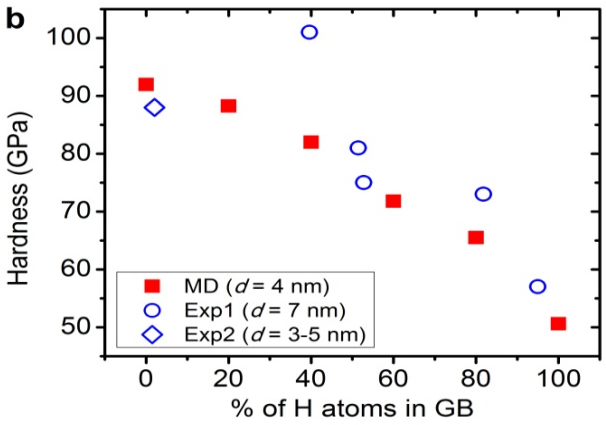
- **Grain boundary (GB) sliding – main deformation mechanism**

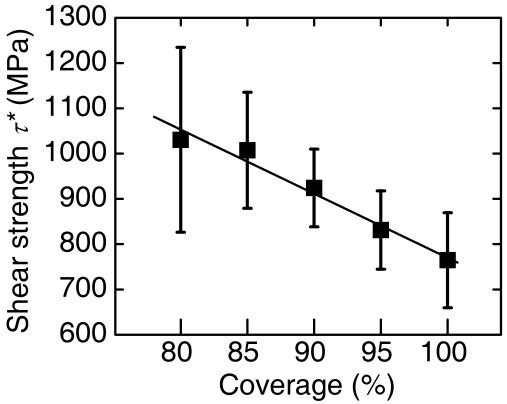




- **Hardness and yield stress are linear with friction (shear strength) of grain boundaries**

- **Hardness of UNCD decreases with increasing H content in GBs**





- **Increasing H coverage of diamond interfaces leads to reduction in friction (shear strength)**
- **This reduction in shear strength at grain boundaries is responsible for reduction in hardness of UNCD**