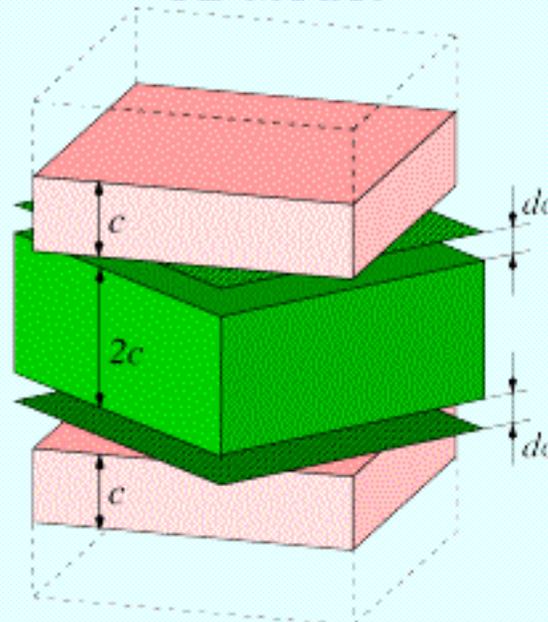


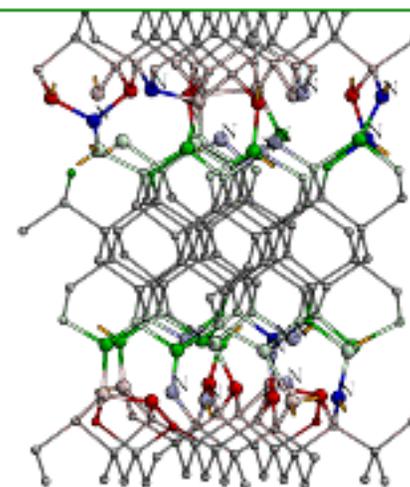
# Electronic Structure of Ultrananocrystalline Diamond Grain Boundaries

- ❖ Twist grain boundaries in diamond result in 40%-50% of three-coordinated atoms in the interface.
- ❖ The nitrogen impurities in UNCD are likely to be in the grain boundaries.
- ❖ Nitrogen can increase conductivity related to carbon  $\pi$ -states. No shallow nitrogen donor for conduction band
- ❖ These results help to understand the unique properties of UNCD.

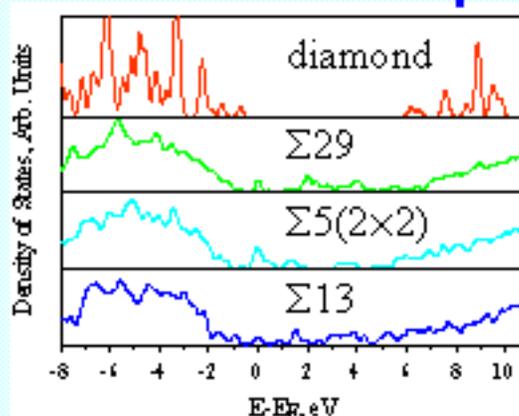
## GB Model



## $\Sigma 13$ grain boundary with high N content



## States in the Gap



## Fermi level shift

