Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

First-principles study of adsorption and migration on the (001) surfaces of cubic BN[1] HIROAKI KOGA, TSUYOSHI MIYAZAKI, National Institute for Materials Science, SATOSHI WATANABE, The University of Tokyo, TAKAHISA OHNO, National Institute for Materials Science — This first-principles study examines the behavior of boron and nitrogen adatoms on the dimer-reconstructed (001) surfaces of cubic boron nitride (cBN), to find low-barrier migration pathways that control the vapor-growth of cBN. Adatom dynamics on the surfaces of wide band gap semiconductors such as cBN (with ∼6 eV gap) and diamond is an uncharted field of surface science: Because these materials have very strong, directional bonds, the adatoms may choose unlikely adsorption sites and migration pathways, to minimize the induced strains. For example, we have found that a N adatom on a N dimer row of cBN(001) migrates using a site-exchange reaction, rather than migrating on the dimer row. The calculated energy barrier for the site-exchange pathway is mere 0.9 eV, in contrast with the large barrier (over 4 eV) of the dimer row pathway. At the meeting, we report such low-barrier pathways on cBN(001), and also discuss a new approach to cBN epitaxy that exploits them.

[1]H. K. is supported by the JSPS Research Fellowships for Young Scientists. This work was in part supported by a Grant-in-Aid from the Ministry of Education, Culture, Sports, Science and Technology.

Hiroaki Koga
National Institute for Materials Science

Date submitted: 15 Jan 2006 Electronic form version 1.4