

# An early stage of *epi* Ge(001)-2x1 oxidation studied by *in-situ* high-resolution synchrotron radiation photoemission

Yi-Ting Cheng (鄭伊婷)<sup>1</sup>, Hsien-Wen Wan (萬獻文)<sup>1</sup>, Chiu-Ping Cheng (鄭秋平)<sup>2,\*</sup>, Jueinai Kwo (郭瑞年)<sup>3,\*</sup>,  
Minghwei Hong (洪銘輝)<sup>1,\*</sup>, and Tun-Wen Pi (皮敦文)<sup>4,\*</sup>

<sup>1</sup>Graduate Institute of Applied Physics and Department of Physics, National Taiwan University, Taipei, Taiwan

<sup>2</sup>Department of Electrophysics, National Chiayi University, Chiayi, Taiwan

<sup>3</sup>Department of Physics, National Tsing Hua University, Hsinchu, Taiwan

<sup>4</sup>National Synchrotron Radiation Research Center, Hsinchu, Taiwan

[d06245005@ntu.edu.tw](mailto:d06245005@ntu.edu.tw)

\*Authors to whom correspondence should be addressed. Electronic addresses:  
pi@nsrrc.org.tw (T. W. Pi), mhong@phys.ntu.edu.tw (M. Hong), raynien@phys.nthu.edu.tw (J. Kwo), and  
cpcheng@mail.ncyu.edu.tw (C. -P. Cheng)

## Abstract

High-resolution synchrotron radiation photoemission (SRPES) was employed to study the atom-to-atom interaction of molecular O<sub>2</sub> and atomic O to *epi* Ge(001)-2x1 at room temperature in the early stage of adsorption. A 30-nm thick Ge *epi*-layer was grown on Ge(001) substrate from Umicore. The *epi* Ge(001)-2x1 grown by molecular beam epitaxy (MBE) has been studied by *in-situ* SRPES, reflection high-energy electron diffraction (RHEED), low-energy electron diffraction (LEED), and scanning tunneling microscopy (STM), showing a flat and long-range order of the *epi* surface. For the *epi* surface, the topmost surface atoms are all buckled, thereby giving rise to up- and down-dimerized configuration. Furthermore, the first subsurface layer also exhibits a distinct peak in the Ge 3d core-level spectrum. An *epi* Ge(001)-2x1 sample was exposed to high-purity O<sub>2</sub> gas at dosages as small as 1 Langmuir (L) and up to 300L. It is found that the O<sub>2</sub> molecules are immediately dissociated without a mediated stage upon reaching the *epi* Ge(001)-2x1 surface. One of the dissociated O atoms removes the Ge up-dimer atom to form the GeO species. The other dissociated O atom inclines to be positioned at the site of the removed Ge up-dimer atom, and bonds with the underneath Ge atom in the subsurface layer. The down-dimer atom and its back-bonded subsurface Ge atom are inert to O<sub>2</sub>. For the atomic O/*epi* Ge(001)-2x1 system, the O adatom is adsorbed between the up-dimer atoms and the underneath subsurface atoms without slicing off any Ge-Ge bond. Similar to the molecular O<sub>2</sub> case, however, the down-dimer Ge atoms and the back-bonded subsurface atoms remain inert to atomic O. The present oxidation study would assist in improving the Ge MOS device growth.

**Keywords** –Oxidation of *epi* Ge(001)-2x1