Chapter 5

Future Perspectives

For the immediate future, the following is the research directions that may be identified as necessary and potentially profitable:

- Nanoindentation-induced deformation of ZnO thin films
- Combination of DAC and nanoindentation techniques to investigate the high-pressure physical mechanisms and characteristics of semiconductors
- Nanomechanical properties of SnAgCu solder by nanoindentation
- Combination of nanoindentation and multiscale simulations to investigate the mechanical deformation of thin films
- Nanowire-based field-effect transistors

The partial topics as follow are proceeding now or will be studied in the future.

A study of nanoindentation-induced deformation mechanisms

Sheng-Rui Jian
Department of Electrophysics, National Chiao Tung University, Hsinchu 300, Taiwan

Mechanical deformation in semiconductor materials is an area of both technological and importance and fundamental interest. The influence of mechanical damage on the properties of semiconductors is crucial in the design and fabrication of nanoscale electronic and optoelectronic devices. Nanoindentation is, in principle, an ideal method for studying mechanical deformation in semiconductors since details of load-displacement curves and hardness parameters can be directly correlated with the induced structural changes.

The works presented in this proposal have addressed the information on the structural changes that occur in materials by using both in-situ and ex-situ techniques to characterize mechanical deformation. The advanced techniques, used in nanoindentation experiments, are able to detect dislocations; however, it is difficult to resolve the atomistic structures and dynamics of dislocations in details. Therefore, molecular dynamics simulations are able to include atomistic effects and is also helpful in providing an understanding of the trajectories of all atoms and has been successfully employed in nanoindentation to obtain valuable insights into atomistic behaviors and to even make comparisons with experiments [1-2]. The subjects listed as follow are proceeding now or will be investigated in future.

Nanoindentation on ZnO thin films

Nanomechanical properties of ZnO thin films were subjected to nanoindentation evaluation. ZnO thin films were created on (c- and a-axis) sapphire and 6H-SiC(0001) substrates by pulsed-laser deposition (PLD) [3-4]. The structure and surface morphology were analyzed by x-ray diffraction (XRD) and atomic force microscopy (AFM). Continuous stiffness measurements (CSM) technique was used in the nanoindentation tests to determine the hardness and elastic modulus of the deposited thin films. Here, the partial experimental results are illustrated in Figs.1-2.

Of note, no pop-in events are observed during loading of all load-displacement curves, as shown in Fig.1. The phenomena are very different from the previous study [5], which displays the multiple pop-in events for the c-oriented bulk wurtzite ZnO.

Pop-in events in single-crystal materials can be attributed to slip along the basal and pyramidal planes and, is different for c-oriented and a-oriented ZnO because of the orientation of the basal plane. In addition, this may be due, in part; pop-in events were attributed to the very poor defect density prior to the nanoindentation tests so that the onset of plasticity requires load sufficient for dislocation nucleation and propagation. In contrast, epitaxial layers are expected to contain more defects like surface steps [6] that are known to facilitate the onset of plasticity [7]. In fact, during this research, no pop-in events are discovered.

In our now/future works, the nanoindentation-induced mechanical damage, focused-ion-beam (FIB) and cross-sectional transmission electron microscopy (XTEM) techniques will be used to identify the deformation mechanisms.

Reference

[1] R. Smith, D. Christopher, S.D. Kenny, A. Richter and B. Wolf, Phys. Rev. B 67 (2003) 245405.

[2] S.R. Jian, T.H. Fang and D.S. Chuu, Appl. Surf. Sci. (2006, ***in press***)

[3] A. Tsukazaki, A. Ohtomo, T. Onuma, M. Ohtani, T. Makino, M. Sumiya, K. Ohtani, S.F. Chichibu, S. Fuke, Y. Segawa, H. Ohno, H. Koinuma and M. Kawasaki, Nature Mater. 4 (2005) 42.

[4] K. Ip, Y.W. Heo, D.P. Norton, S.J. Peatron, J.R. LaRoche and F. Ren, Appl. Phys. Lett. 85 (2004) 1169.

[5] S.O. Kucheyev, J.E. Bradby, J.S. Williams, C. Jagadish and M.V. Swain, Appl. Phys. Lett. 80 (2002) 956.

[6] G. Patriarche, F. Glas, G.L. Roux, L. Largeau, A. Mereuta and J.L. Benchimol. J. Cryst. Growth 221 (2000) 12.

[7] S. Brochard, J. Rabier and J. Grillhe, Eur. Phys. J. AP 2 (1998) 99.

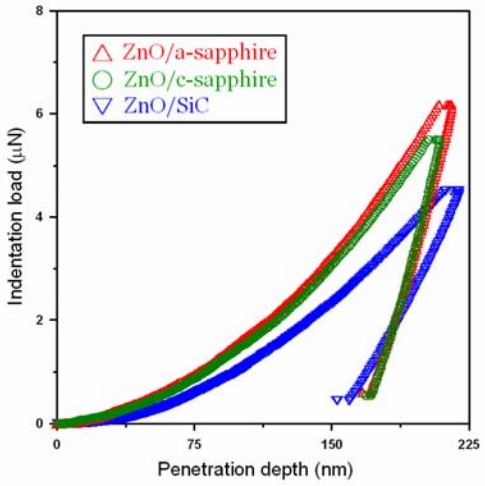

Fig.1. Typical load-displacement curves measured during nanoindentation of ZnO thin films on three various substrates.

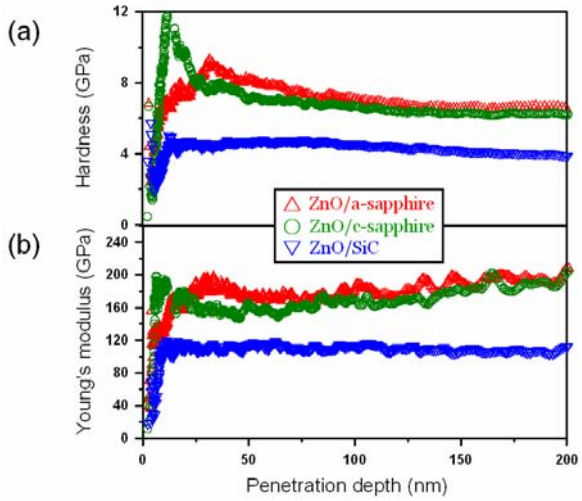

Fig.2. (a) Hardness and (b) Young's modulus of ZnO thin films on three various substrates plotted as a function of the penetration depth.

Atomistic modeling of metal thin films under nanoindentation

Parallel molecular dynamics simulations are performed for this study of dislocation nucleation and evolution in Ni metallic thin films under nanoindentation. Here, the partial experimental results are illustrated in Fig.1. The dimensional scales of the simulated model are approximately $20\times20\times4$ nm^3. The indenter tip has the conical shape with a diameter of 6 nm and height of 3 nm.

In our present simulations, the interatomic forces of the potential functions in the whole system are described by the tight-binding potential, as following:

$$\Phi_{total}=\sum_{i=1}^{N}\Phi_{ij}=\sum_{i=1}^{N}\left\{-\left[\sum_{j}\xi^2\exp\left(-2q\left(\frac{r_{ij}}{r_o}-1\right)\right)\right]^{1/2}+A\exp\left[-p\left(\frac{r_{ij}}{r_o}-1\right)\right]\right\} \quad (1)$$

where the subscripts i and j represent atom i and atom j, respectively; ξ is an effective hopping integral, r_{ij} is the distance between atoms i and j, and r_0 is the first-neighbors distance. The total band energy is characterized by the second moment of the d-band density of state and is shown in the first part of potential function. Meanwhile, the second part reveals a modified form of the original tight-binding potential. The free parameters of A, ξ, p and q are fitted to the experimental values of cohesive energy, lattice parameters and independent elastic constants for the system.

The interaction force F_i on atom i is derived from the Eq.(1), can be expressed as

$$F_i=-\sum_{j\neq i}^{N}\left(\frac{\partial\Phi_{ij}}{\partial r_{ij}}+\frac{\partial\Phi_{ij}}{\partial r_{ij}}\right)=m_i\frac{d^2r_i(t)}{dt^2} \quad (2)$$

where m_i is the mass of atom *i*, *r* is the position of atom *i*, and *N* is the total number of atoms. Using Eq.(2), the resultant forces of each individual atom can be calculated at the each time step. The tight-binding potential for the interatomic forces in our simulated models has been employed in the related research in MD simulations [1]. Also, the numerical method and periodic boundary condition can be found in Ref.2-3.

Our present results indicated that the evidence of permanent deformation mediated through the glide during nanoindentation, as shown in Fig.1. Dislocation nucleations occurred inside the material near the top of surface and generated loops in the {111} slip planes. As the indentation process advanced, the indentation-induced energy release because of the emission of dislocations, leads to the overall re-increase of indentation load during this period of gliding until the next partial dislocation is triggered to fully grow. It is interesting to note that the permanent formation of slip planes and piling-up on the subsurface layers of Ni are also observed, indicating that local inhomogeneous deformation occurred and, its mechanism is one of nucleation and propagation of new shear bands during nanoindentation.

In our now/future works, the multiscale (molecular dynamics simulation combined with finite element method) simulations will take into account for the nanoindentation-induced deformation mechanisms on various materials (such as metals, semiconductors, ceramics and alloys and etc) in detail at the atomic level.

Reference

[1] F. Cleri and V. Rosato, Phys. Rev. B 48 (1993) 22.

[2] J.M. Haile, *Molecular Dynamics Simulation: Elementary Methods* (Wiley, New York, 1992)

[3] S.R. Jian, T.H. Fang and D.S. Chuu, Appl. Surf. Sci. (2006, ***in press***)

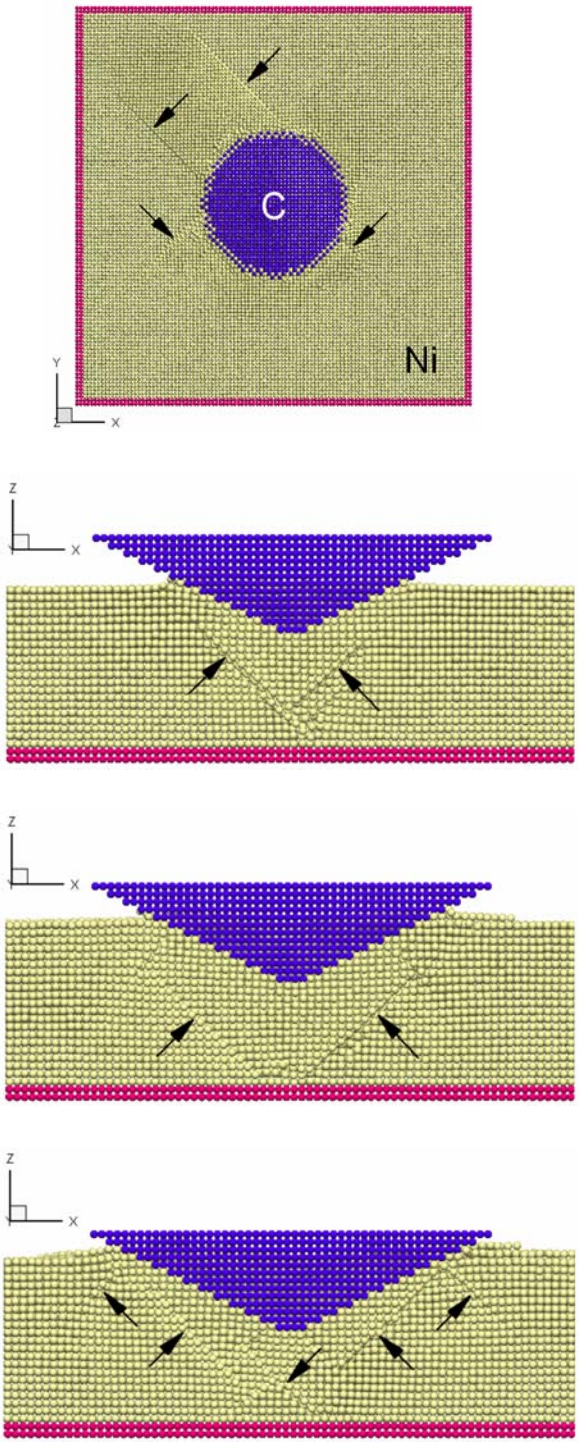

Fig.1 Top and the cross-sectional views of (010) plane of MD simulation surface showing the dislocation loops gliding and nucleated on {111}<110>-slip systems.

SiGe-based Nanowire Field-Effect Transistors

Sheng-Rui Jian
Department of Electrophysics, National Chiao Tung University, Hsinchu 300, Taiwan

I. *Introduction*

Silicon nanowires (SiNW) [1] and carbon nanotubes (CNT) [2] have attracted much attention for their potential use in the fabrication of nanoelectronics devices because of their one-dimensional, high surface to volume and unique characteristics [3-4]. For these applications, the structures made of SiNW or CNT are field-effect transistors (FET) with direct metal contacts forming the source and drain [5-6]. Nevertheless, there has little experimental study on the characterizations of nanoscale channel SiGe-based NWFET up to now.

In our present work, molecular beam epitaxy (MBE) was used to grow the SiGe quantum well structures and focus ion beam (FIB) was used to fabricate the nanowire structures. Next, the electrical characterizations of SiGe-based NWFET will be investigated in our future work.

II. *Experimental details and Our present results*

The process flow was shown in the Fig.1. The sample was grown to form the quantum well structure by solid source molecular beam epitaxy (MBE). First, low temperature (LT) silicon buffer layer was grown at the temperature of 400 ^{o}C on a *p*-type Si

substrate with <100> crystal orientation and a resistivity of 1-10 Ωcm. Fully-relaxed $Si_{1-x}Ge_x$ layer with a thickness of 300 nm was grown at 550 ^oC on LT Si layer. And then silicon channel layer under bi-axial tensile strain with a thickness of 10 nm was grown on the relaxed $Si_{1-x}Ge_x$ layer. At the same time, Sb with concentration of 10^{17} cm^{-3} was doped into silicon channel layer. Finally, $Si_{1-x}Ge_x$ capping layer with 5 nm was capped on the silicon channel layer to form the quantum well structure. After the epitaxy process, two optical photo-lithography procedures were used to form the contact and mesa. Channel with a width of 10-30 nm was formed by focus ion beam (FIB), as illustrated in Fig.2. The liquid phase deposited SiO_2 [7] with a thickness of 20 nm was grown on the surface of the device to form the gate insulator. Then, the gate contact metal was evaporated on the gate insulator.

Now, the SiGe-based nanowire structures have been successfully fabricated. The electrical and physical properties of SiGe-based NWFET will be measured and investigated in our future work.

Reference

[1] S.M. Koo, A. Fujiwara, J.P. Han, E.M. Vogel, C.A. Richter and J.E. Bonevich, Nano Lett. 4 (2004) 2197.
[2] Y. Cui and C.M. Lieber, Science 291 (2001) 851.
[3] X.F. Duan, Y. Huang, Y. Cui, J.F. Wang and C.M. Lieber, Nature 409 (2001) 66.
[4] E.D. Minot, Y. Yaish, V. Sazonova, J.Y. Park. M. Brink and P.L. McEuen, Phys. Rev. Lett. 90 (2003) 156401.
[5] S.J. Trans, R.M. Verschueren and C. Dekker, Nature 393 (1998) 49.
[6] Y. Cui, Z. Zhong, D. Wang, W. Wang and C.M. Lieber, Nano Lett. 3 (2003) 149.
[7] C.F. Yeh, S.S. Lin, T.Z. Yang, C.L. Chen and Y.C. Yang, IEEE Trans. Electron Devices 41 (1994) 173.

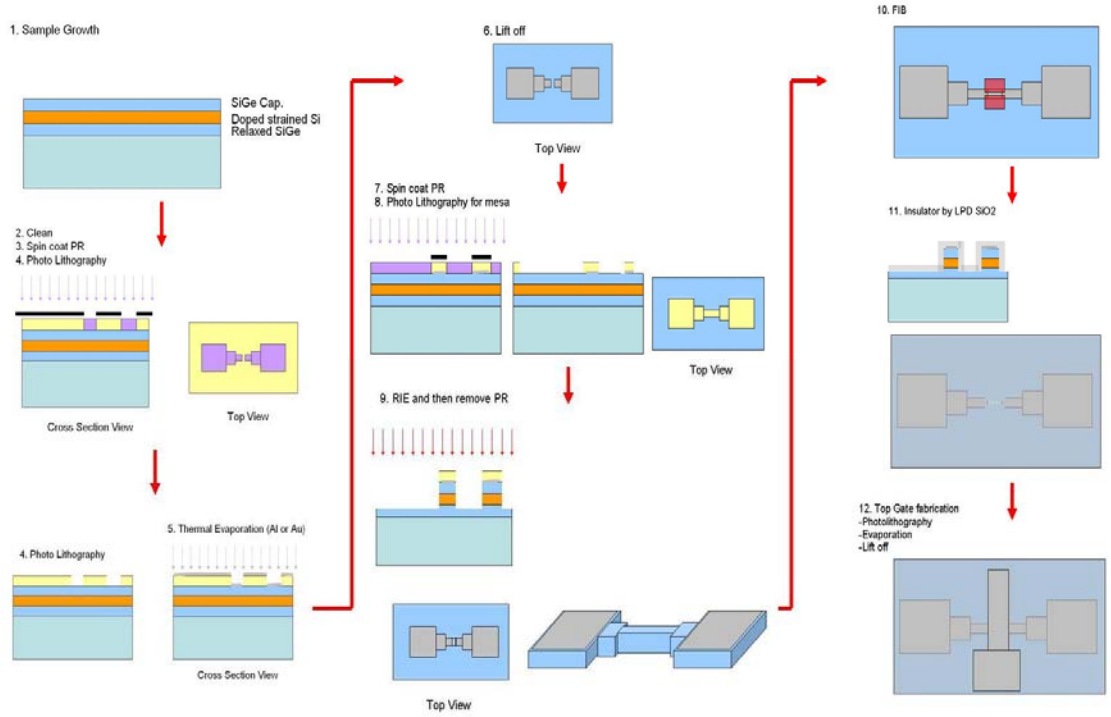

Fig.1. Process flow of fabrication of SiGe-based nanowire device.

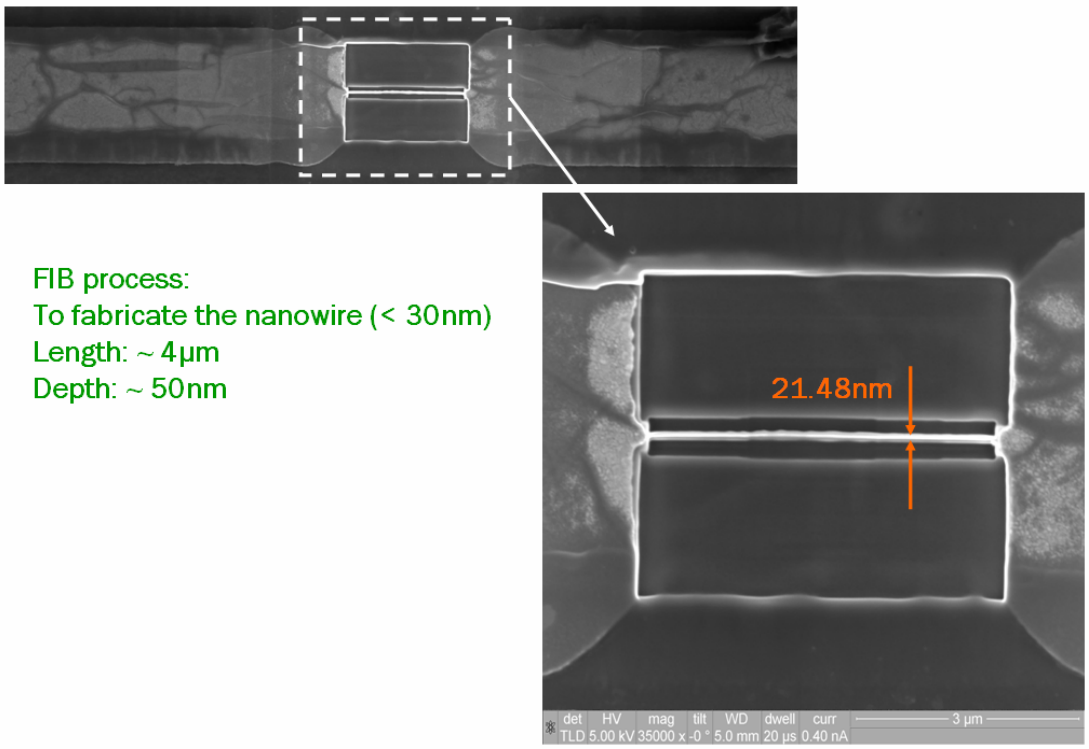

Fig.2. SiGe-based nanowire structure fabricated by FIB.

Parts of this chapter have been submitted in:

1.) S.R. Jian,

"Nanomechanical characterizations of ZnO thin films"

submit to ***Journal of Physics D: Applied Physics*** (2006);

2.) S.R. Jian, W.P. Huang, C.M. Lin, J.Y. Hsieh, D.S. Chuu and H.H. Cheng,

"Localized electrochemical oxidation of *p*-GaAs(100) using an atomic force microscopy with carbon nanotube probe"

submit to ***Nanotechnology*** (2006);

3.) C.H. Chien, C.T. Wang, W.J. Lee, Y.C. Lo, S.P, Ju, J.C. Huang and S.R. Jian,

"Atomic-scale simulations on the material characteristics of crystalline metals and amorphous alloy by nanoindentation"

submit to ***J. Appl. Phys.*** (2006).