演 題 : **Mechanics Meets Electronics in Nanoscale: The Mystery of Current Spike and Nanoscale Confinement**

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場 所 : フロンティア応用科学研究棟セミナー室 1
要 旨 :

Introduction

One of the primary areas of research concerns the discovery, understanding, and control of the drastic property differences between nanoscale and microscale volumes of material. It recently became recognized that the deformation of nanoscale volumes contrasts the classical perception of microscale deformation, where dislocations are the primary mode of deformation (e.g., [1-3]). Our results combine localized electrical measurements and nano-mechanical probing to demonstrate that this need not always be true [4]. Instead of dislocation activity, the onset of permanent deformation at the nanoscale may simply be the result of a transition from one crystal structure to another. This correlation is solidified by our atomistic calculations [4-5] which prompted us to further our consideration to semiconductor nanoparticles [6] (see Fig. 2).

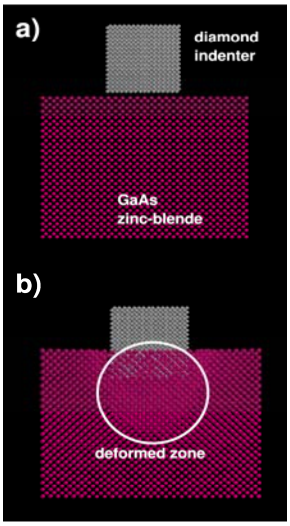

Fig. 1. The schematic of nano-indentation process into the (001) plane of GaAs crystal modelled by MD-simulation.
The picture illustrates the atomic arrangement prior to and in course of the penetration of a diamond cube indenter into GaAs cluster.

Silicon nanoobjects exhibit unique electrical, optical as well as piezoelectric and thermoelectric properties, which opens a broad range of their applications. Extensive study of the electrical and optical properties of silicon nanoparticles somewhat overshadows their mechanical properties. Given the evidence of the significant impact of crystal imperfection on the functional properties of nanovolumes, understanding their response to applied stress draws growing interdisciplinary interest [7]. The introduction of the “nanoscale confinement” parameter [6] (never explicitly taken into account so far for size-dependent phenomena) resolves dilemma noted by the earlier studies and offers avenues to a nanoscale device design.

Current spike - the signature of phase transition

One of the fundamental questions in materials science concerns the nature of deformation of solids [8]. The onset of plasticity is traditionally understood in terms of dislocation nucleation and motion. A study of nanoscale deformation has proven that initial displacement transient events occurring in metals are the direct result of dislocation nucleation [1-3].
Here we show that nanoscale deformation may simply be due to transition from semiconductor to metal crystal structure as confirmed in the case of GaAs [4-5]. Using a novel conductive nanoindentation technique, we discovered the essential link between this electrical transport

phenomenon and the mechanical transient (pop-in) exhibited by GaAs exclusively during nanoscale deformation (see Fig. 2).

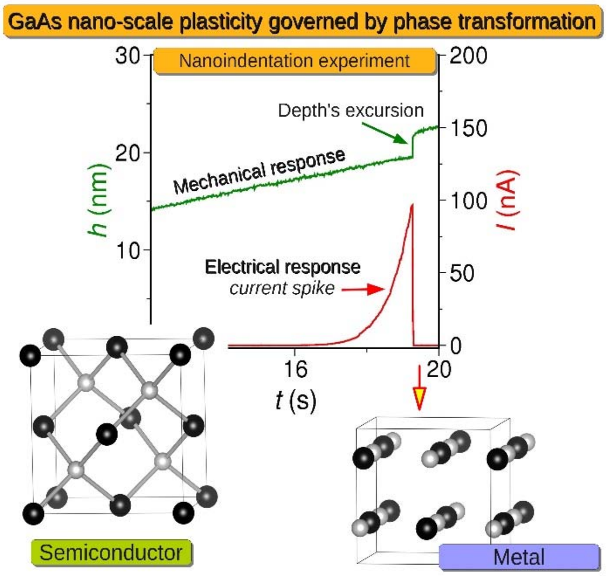

Fig. 2 The result of *in situ* nanoscale electrical resistivity measurements of the (100) GaAs crystal demonstrate the peculiar electric current spike (reverse bias) that appears simultaneously with pop-in event during indentation with conducting tip. The Current-Time curve recorded during elastic nano deformation proves leaking junction and immediately after pop-in event –the restoration of a perfect Schottky barrier. The phenomenon we named the "Current Spike" is clearly visible, and its explanation relies heavily on quantum calculations [4].

Our molecular dynamics (MD) modeling and *ab initio* calculations of the processes that occur in a tiny crystal volume right under the loaded tip, brought into light the new scenario (see Figs. 1 and 2). The pop-in incident that solely reflects a nanoindentation-induced phase transformation, is accompanied by no dislocation nucleation. We reveal the transition of GaAs from zinc-blend to rocksalt-like structure hitherto unreported for the crystal deformed by nanoindentation. The appearance of new phase at the point marked by pop-in event was documented by visualization of the atomic positions and singularities in the structural correlation functions [4-5]. This correlation leads to the conclusion that a previously unseen phase transformation is the fundamental cause of nanoscale plasticity in GaAs [4].

Indeed, anyone wishing to project to nanoscale, even with such classic phenomena as elastic or plastic deformation, will inevitably look to the atomistic approach for answers. The presented results lead to a major shift in our understanding of elastic-plastic transition [5] as well as inherent Schottky barrier formed in semiconductors under local high pressures [4]. We expect this to hold true for a variety of other covalently bonded materials, ultimately leading to an increased understanding of nanoscale plasticity and advances in pressure-sensing, pressure-switching, and future phase-change applications.

Nanoscale confinement of stressed volume

Nanoparticles are everywhere: in cosmetics and for manufacturing transistors. In bulk, many materials like silicon are as brittle as glass. In nanoparticle shapes one billionth the size of a window pane, they deform plastically. That is, you can compress them to half their size and they won't shatter. How can this happen? Atom by atom rearrangements are followed in the computer and experimentally by squeezing small spheres while simultaneously visualizing them under the electron microscope. Such mechanically induced shape changes occur by different processes depending on size.

Here we present atomistic calculations and supporting experimental results revealing a heretofore unknown dislocation-driven mechanism in Si nanoparticles. Molecular Dynamics simulations match the experimental data exhibiting striking contrast to deformation of bulk Si surface. The observed behavior is examined in the framework of the dilemma concerning dislocation [1-3], or phase-transformation [4-5,9] origin of the incipient plasticity in nanoscaled solids. MD-calculations and supporting experimental results reveal that plasticity onset in Si nano-spheres below 57 nm radius is governed by dislocation-driven mechanisms, in striking contrast to bulk Si where plasticity is dominated by phase transformations [6,8]. With the broad implications for nanotechnology, we establish previously unforeseen role of 'nanoscale confinement' governing a transition in mechanical response from "bulk" to 'nanovolume' behaviour (refer to Fig. 3).

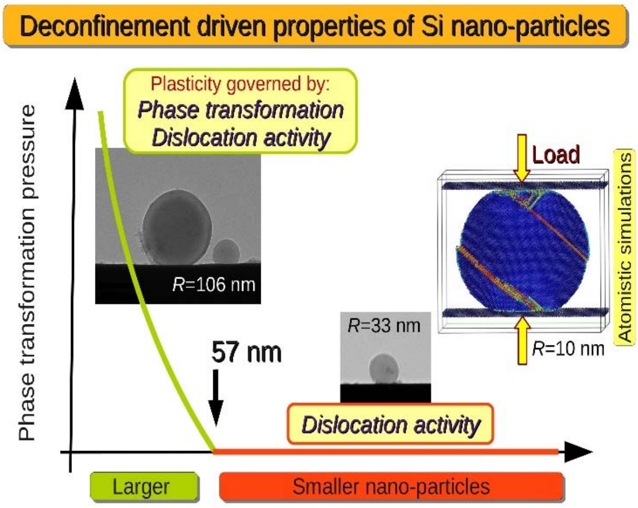

Fig. 2 Molecular dynamics calculations and supporting experimental results reveal that plasticity onset in Si nano-spheres below 57 nm radius is governed by dislocation-driven mechanisms. These findings are in contrast to bulk Si, where incipient plasticity is dominated by phase transformations. The shift from transition-driven to dislocation-governed incipient plasticity is caused by progressing deconfinement of stressed Si nanovolume.

Our findings reinforce previous studies proposing that the onset of plasticity in nanoscale volumes is driven by the crystallography and geometry [1-5,8-9]. It is a very encouraging demonstration of the way in which nanomechanics may contribute to electronic and optoelectronic developments. This understanding benefits processing of nano-structures for electronic, magnetic and optical devices as well as biomedical applications including drug delivery and biosensors as indicated by Cross [7]. Furthermore, it provides a repeatable means for generating crystal imperfections which dramatically impact functional properties and biocompatibility.

The succinct explanation of this topic affects future nano-devices and offer promise for ultraviolet photo detectors, 'laser on a chip' devices, drug delivery and biological markers [7-8].

References

[1] Li, J., Van Vliet, K.J., Zhu, T., Yip S. & Suresh, S., *Nature* **418**, 307 (2002).

[2] Schuh, C.A., Mason, J., & Lund, A., *Nature Materials* **4**, 617 (2005).

[3] Kiener, D., Hosemann, P., Maloy, S. & Minor, A.M. *Nature Materials* **10** 608 (2011).

[4] Nowak, R., Chrobak D. *et al.*, *Nature Nanotechnology* **4**, 287 (2009).

[5] Chrobak, D., Nordlund, K. & Nowak R., *Phys. Rev. Lett.* **98**, 045502 (2007).

[6] Chrobak, D., Nowak, R., *et al.*, *Nature Nanotechnology* **6**, 480 (2011).

[7] Cross G.L.W. *Nature Nanotechnology* **6** 467 (2011).

[8] Nowak, R., Yoshida, F., Chrobak, D. et al., *Encyclopedia of Nanoscience and Nanotechnology*, Am. Sci. Publ., 313-374 (2011).

[9] San Juan, J., Nó, M.L. & Schuh, C.A. *Nature Nanotechnology* **4**, 415 (2009).

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