



Professor Alberto M. Cuitiño
American Academy of Mechanics
School of Engineering
Rutgers University
98 Brett Road
Piscataway, NJ 08854-8058

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SELECTION OF THE EDITOR

Understanding How Nanocrystalline Metals Deform

Kevin J. Hemker

Department of Mechanical Engineering, Johns Hopkins University, Baltimore, MD
21218–2681, USA. E-mail: hemker@jhu.edu

The functionality and overall reliability of emerging micro- and nanoscale devices are closely tied to the mechanical properties of the nanocrystalline materials from which they are constructed. Most engineering materials are composed of thousands if not millions of tiny crystallites (called grains), and it is now widely recognized that reducing the grain size of a material will result in greatly increased strength and hardness. What is not currently understood is how these nanocrystalline materials accommodate plastic deformation—the phenomenon in which materials permanently change shape. The experiments described by Budrovic *et al.* (1) are exciting because they provide a new avenue for characterizing the deformation behavior of nanocrystalline metals.

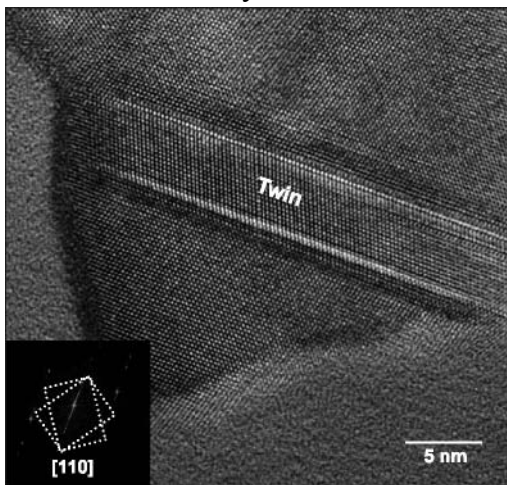
Ensuring the reliability of next-generation microelectromechanical systems (MEMS), nanoelectromechanical systems (NEMS), integrated circuits, and micro and nanoscale devices in general will require a fundamental description of their mechanical behavior. To be truly predictive, this description must be based on a solid understanding of operative deformation mechanisms. The fact that these mechanisms have not been clearly identified for nanocrystalline materials, however, is currently exacerbated by the limitation that many of the plasticity models that were developed to describe conventional coarse-grained materials are known to break down at these reduced length scales.

The importance of dislocation activity, grain boundary sliding, diffusive processes, fatigue, and fast fracture have been addressed in

microcrystalline metals and alloys, but the relative importance of these processes has yet to be established in their nanocrystalline counterparts. Methodologies used to characterize deformation behavior in microcrystalline metals have also been used to study nanocrystalline metals, but difficulties associated with the proliferation of intergranular regions and the inherent characteristics of the deformation processes have seriously hindered these efforts. The results obtained by Budrovic *et al.* (1) using in situ peak profile analysis of samples being deformed in the Swiss synchrotron Light Source provide a unique thumbprint of plastic deformation in nanocrystalline nickel. As such, these experiments provide a valuable complement to ongoing theoretical and experimental studies of deformation mechanisms in nanocrystalline materials.

X-ray diffraction profile analysis is a well-established technique for indirect characterization of dislocation substructures. Peak broadening occurs as a result of both limited scattering volume and the presence of inhomogeneous lattice strains. In microcrystalline metals the latter is often related to dislocation storage, and the shapes of x-ray peaks have been used to deduce indirect measures of dislocation densities, arrangement parameters, dipole polarization, and dislocation character (2). The results for coarse-grained copper reported by Budrovic *et al.* (1) are in agreement with previous studies, but their discovery that peak broadening in nanocrystalline nickel is fully recovered upon

unloading was not expected, and this surprising result has two important implications. First, it implies that dislocation activity is fundamentally different in nanocrystalline nickel. Second, the peak broadening that occurs when the sample is loaded provides an indirect measure of the as-yet undiscovered process, or processes, that lead to plastic deformation in nanocrystalline nickel.



Nanoscale deformation. High-resolution transmission electron micrograph of a twin in deformed nanocrystalline aluminum (10). This atomic resolution image illustrates the mirror symmetry between the twin and the matrix. The presence of the twin and the fact that it extends from one side of the grain to the other are unique to nanocrystalline aluminum.

In metals with grain sizes of greater than 100 nm, strengthening at reduced grain sizes is attributed to the pile-up of dislocations at grain boundaries and is modeled by the semi-empirical Hall-Petch relation. The physical basis for this model breaks down as grain size is reduced to several tens of nanometers, and measured values of the flow strength have confirmed that this relation cannot be extrapolated to nano-crystalline grain sizes (3, 4). Grain boundaries are highly effective dislocation sinks and sources, and it is generally acknowledged that traditional dislocation sources cease to operate when the metals become nanocrystalline. Post-mortem transmission electron microscope (TEM) observations of deformed nanocrystalline metals have failed to uncover any evidence of

dislocation activity or debris characteristically observed in microcrystalline metals (5, 6). The building consensus that deformation processes are different in nanocrystalline metals is further supported by Budrovic's measurements (1), because observation of fully reversible peak broadening would not be compatible with dislocation plasticity involving dislocation tangling and storage. Molecular dynamics (MD) simulations have been used to study the atomic-scale processes that occur during the plastic deformation of polycrystalline aggregates of nanocrystalline grains (7-9). Although these simulations must be conducted at extremely high strain rates ($\sim 10^7 \text{ s}^{-1}$), they have provided useful insight about the deformation processes that may occur in nanocrystalline metals. The simulations suggest that nanocrystalline metals accommodate externally applied stresses by means of grain boundary sliding and the emission of partial dislocations that run across the grain and are absorbed into the opposing grain boundary (7-9). The extremely short lifetime of these emitted and reabsorbed dislocations explain why they are not directly observable by TEM and why they do not form dislocation debris that would lead to permanent x-ray peak broadening. The MD simulations are also in good agreement with recent experimental observations of twinning and stacking fault deformation in crushed and indented nano-crystalline aluminum (see the figure) (10). Twins and stacking faults are formed by partial dislocation motion. The fact that twins were not present in the as-deposited films and can be directly related to plastic deformation has been used to underscore the transition that occurs when grain size decreases to tens of nanometers (10).

The MD simulations also suggest that grain boundary sliding and partial dislocation emission are triggered by atomic shuffling and, to a lesser extent, free volume migration in the grain boundaries (4). These dynamic, atomic-scale processes would be nearly impossible to image with TEM, but because they change the structure of the grain boundaries, it is possible that they are contained in the peak-broadening measurements of Budrovic et al. (1). The

evidence that diffraction peaks are sharpened as a result of plastic deformation [figure 3A in (1)] is one indication of structural rearrangement in the grain boundaries. Results like this are exciting because they demonstrate that in situ x-ray peak profile analysis can be used to collect indirect information about atomic-scale intra- and intergranular deformation processes in nanocrystalline materials. With the development of more quantitative analysis techniques and improved structural models, this methodology can be expected to play an important role in uncovering and defining nanostructure-mechanical property relations in nanocrystalline metals.

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AAM NEWS

2005-2006 Founders Prize and Grant Awarded

The winner is **Vivek Verma**, a graduate student at the Pennsylvania State University, the Prize awarded for his essay, "Progress through Mechanics: *Biomolecular Motors*". The Prize check for one thousand dollars will be presented by President Michael Paidoussis at the ASME Applied Mechanics Dinner. The recipient is also entitled to expenditures for equipment of up to nine thousand dollars to support his research program. The Founders Prize and Grant is sponsored by the Robert M. and Mary Haythornthwaite Foundation (www.haythornthwaite.org).

Progress through Mechanics: *Biomolecular Motors*

Vivek Verma

Department of Engineering Science and Mechanics, The Pennsylvania State University
188 MRI, 230 Innovation Blvd, University Park PA 16803
E-mail: vzv103@psu.edu

All living creatures are made up of cells that have the ability to replicate themselves in a repetitive process called cell division. As these cells mature and divide into two there is an extensive movement of cellular components. In order to perform this essential task that sustains life, cells have evolved machines composed of proteins to perform this function.

Biological motors, such as kinesin and dynein[1-3], transport intracellular cargo and

position organelles in eukaryotic cells via unidirectional movement on cytoskeletal tracts called microtubules. Microtubules are made up of cylindrical polymers of the protein tubulin that typically have a diameter of 25 nm and are several micrometers in length[4]. In order to transport cargo or reorganize organelles along these microtubules, molecular motors convert chemical energy from the hydrolysis of adenosine triphosphate(ATP)[1] into mech-

anical energy. For example, kinesin can exert a maximal force of 6 pN[2] and can be immobilized on surfaces with densities of $\sim 10^3$ motors/ μm^2 [5] delivering a cumulative force on the order of $\text{nN}/\mu\text{m}^2$. These motors have been purified from cell cultures and quantified for standards such as velocity and power stroke per cycle. The ability to use biological motors *in vitro* makes them strong candidates for high-efficiency nanoengines. These are nature-made motors with a certain degree of robustness and a very high specificity to the types of cargos to which they bind. These motors are complete in themselves with many opportunities to use them for making different devices and structures. Some applications of biomolecular systems are envisioned below.

(a) Powering switchable devices: Nanofabrication processes have enabled the production of devices and structures with dimensions less than 10 nm. Motor technologies, based on silicon or other material systems, useful for powering such devices are not available, thus directing attention towards hybrid systems integrating synthetic molecules or biological motors [6-8]. Motors can easily be purified from cell cultures and have a high-energy conversion efficiency ($\sim 50\%$). Earlier studies have proved that the forces produced by the biomolecular motors are sufficient to power micro/nano electro-mechanical system (MEMS/NEMS) devices. For instance, if a micro gear with microtubules oriented on the cogs of the gear is placed on a bed of motors, it will start to rotate. Similarly, micropumps and microcantilevers powered by molecular motors have also been envisioned.

Microtubules have directional polarity, the fast polymerizing side is called the plus end and the other side is called the minus end. Kinesin moves towards the fast growing side of microtubules and dynein walks towards the minus end. These motors can be patterned juxtaposed on microfluidic channels, so that a device patterned with microtubules can be in contact with only one kind of motor. Changing pressure in the channels will allow a second type of motor to come in contact with a microtubule and the device will change the

direction of motion. This will result in a switchable device.

(b) Directed self assembly: Microtubule based biomotors can be used for directed assembly of synthetic nanostructures. The fact that motor proteins walk unidirectionally on microtubules can be used for such self assembly. For this kind of self assembly all microtubules should be aligned with the plus end on one side and minus end on the other to the substrate. Motor proteins functionalized with the synthetic molecules can then be incubated on the substrate. Motors, e.g. kinesin, attached to synthetic molecules in solution can bind to the microtubules and walk along to the plus end. This way, kinesin will carry the synthetic molecule to the other end. The atomic force microscope (AFM) can also be used to assemble molecules but the process is very slow because the AFM tip can position only one particle at a time. On the other hand, there will be millions of motors working in concert to assemble a nanostructure, resulting in a faster process.

(c) Protein separation and identification: Kinesin and related motor proteins can be mutated so that they bind to specific cargos. This property can be employed to separate a particular protein from a protein mixture. Modified motors can be incubated in a mixture of proteins so that they bind to the desired protein. The motors will then bind to microtubules, walk along them and carry out the separation.

The biggest challenge in using biological motors is the lack of interdisciplinary expertise. To engineer systems using biological proteins it is necessary to pattern proteins and align microtubules at specific locations. To facilitate this complicated process, combined efforts from cell-biology, physics, chemistry, microelectronics and nanotechnology are needed. The lack of communication amongst the different disciplines is one of the main issues slowing the application of biomolecular motors in practical life.

Molecular motors offer several applications from devices to molecular self-assembly. There are innumerable ways these motors can be used, from transporting molecular shuttles to organizing molecules on surfaces. These motors can also help us understand certain cell functions in a better way. For example, the cell's ability to transport a specific cargo to a particular location using different biomolecular motors encourages us to make devices that will separate different molecules. Understanding how cells orient microtubules during cell division and the various motors responsible for different tasks that eventually lead to cell division may one day hold the key to fighting cancer. It is well known that cancer cells divide in an uncontrolled manner. And just like any other cell division, biomotors are also required here. Research is in progress to investigate the role of each type of kinesin and dynein so that cell division is better understood. This type of research will eventually help in discovering the motors critical for cancer cell growth. This way, specific motors can be targeted within cancer cells which will restrict cancer cell division and hence the growth of cancer.

With increasing demands for innovative ideas in micro/nanoscale devices, nature has presented us with a wide opportunity to utilize these motors *in vitro*, to study their role in important cellular processes such as mitosis, and to understand their implications in certain human diseases such as cancer.

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A doctoral degree or equivalent in a relevant area of science or engineering is required. Senior applicants must have a distinguished scholarly record with international visibility. Prior experience working within a multidisciplinary team is desirable, since such research is highly valued in ESM. A large number of faculty members from other departments are affiliated with ESM. Our faculty members work closely with the School of Biomedical Engineering and Sciences (www.sbes.vt.edu) and the Macromolecular and Interfaces Institute (www.mii.vt.edu). Virginia Tech is also home to System X, a world-class terascale computing facility (www.tcf.vt.edu).

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