Yield Strength of MgO in Nanocrystals

C. Chen,[1] J. Chen,[1] J. Zhang,[2] D.J. Weidner,[1] Y. Wang[3]
[1]Mineral Physics Institute, State University of New York (SUNY) at Stony Brook, NY, U.S.A.
[2]Los Alamos Neutron Science Center (LANSCE), Los Alamos National Laboratory, Los Alamos, NM, U.S.A.
[3]GSECARS, The University of Chicago, Chicago, IL, U.S.A.

Introduction

Nanocrystalline materials have been attracting rapidly increasing interest in the last decade, and they hold the promise of revolutionizing traditional materials design in many applications by means of atomic-level structural control to tailor engineering properties. New properties, phenomena, processes, and functionalities have been discovered in nanoscale-size materials (between isolated atoms or molecules and bulk materials; i.e., 1-100 nm). As opposed to the microscale, the nanoscale is not just another step toward miniaturization but rather a qualitatively new scale, since meeting this size constraint often produces qualitatively new behavior. We now understand, in a general way, that when the sample size, grain size, or domain size becomes comparable with a specific physical-length scale (e.g., the mean free path, the domain size in ferromagnets or ferroelectics, the coherence length of phonons, or the correlation length of a collective ground state like superconductivity), the corresponding physical phenomenon will be strongly affected.

Although such changes in behavior can be the dominant effects in nanoscale structures, we still have little experience or intuition for the expected phenomena and their practical implications. In order to understand the mechanical property of nanocrystals, we measured the yield strength of nanosize MgO by using a multi-anvil press and x-ray diffraction at the sector 13 bending magnet beamline at the APS.

Methods and Materials

The nanosize (average 30 nm) crystalline powder of MgO sample is purchased from Nanopowder Enterprises Inc. The powder sample is loaded in a 1-mm-diameter cylindrical chamber. A layer of NaCl powder is also loaded in the sample chamber for internal pressure calibration. The sample chamber is placed between two strip heaters made of Re foil in an octahedral pressure medium. A thermocouple (W5% Re-W23% Re) is inserted into the sample chamber for measuring the sample temperature. The sample is compressed to 14 GPa at room temperature stepwise. Energy-dispersive x-ray diffraction patterns are collected at each pressure.

The average deviatoric stress in the powder sample, generated as a result of grain-to-grain contacts during the loading, is derived from the peak broadening in the diffraction patterns. The grain size of the sample is also monitored through the diffraction peak broadening. Contributions of the stress and grain size to the peak broadening are described by the following equation:

$$[\beta(E)]^2 = \left(\frac{K(\frac{1}{2}hc)}{L \sin\theta_0} \right)^2 + (2eE)^2 \qquad (1)$$

where $\beta(E)$ is the x-ray diffraction peak broadening at the photon energy of E, K is the Scherrer constant, h is the Planck's constant, c is the velocity of light, L is the average grain size, θ_0 is the Bragg angle, and e is the average strain in the sample powders. The grain size and strain contributions are separated by plotting $[\beta(E)]^2$ as a function of E^2. The experimental data are presented by a linear relation in the plot with a slop of $4e^2$ and a Y-intercept of $(1/2\ Khc/L\ \sin\theta_0)^2$. The average strain in the powder sample and average grain size can be derived by fitting experimental data into a linear equation. The stress that the sample experiences during the experiment is obtained by multiplying the strain by Young's modulus of the sample.

Results and Discussion

Figure 1 shows a plot of peak width versus photon energy in the diffraction patterns of MgO and NaCl taken at ambient conditions. The NaCl data serve as a standard for sampling the instrumental broadening. Since both the MgO and NaCl sample are measured at a stressfree state, the two sets of data show an identical slope. The data from the MgO sample produce a bigger Y-intercept, indicating a smaller grain size than that of the NaCl sample. The grain size of NaCl (~microns) contributes very little to the peak broadening. Broadening due to the grain size of the MgO sample is obtained by subtracting the instrumental broadening, and the grain size is derived according to Eq. (1). Measured average grain sizes of the MgO sample at different pressures are plotted in Fig. 2, which shows that the grain size is kept in nanometer-size in this pressure range and at room temperature. There is a slight reduction in grain size during the loading. Figure 3 shows the stresses that the sample experiences as a function of loading (pressure). The stress increases

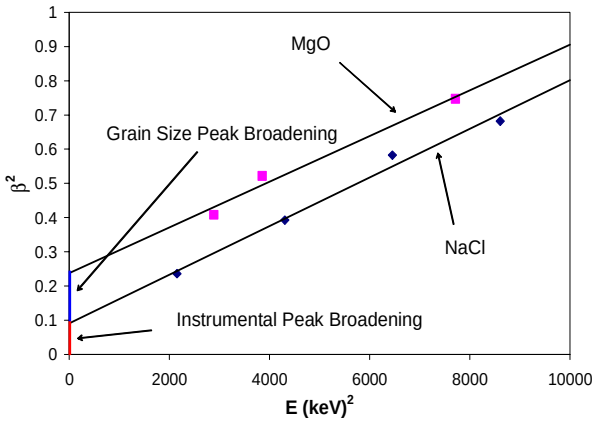

FIG. 1. Peak broadening (β^2) versus photon energy E^2 for diffraction pattern of MgO and NaCl at ambient conditions.

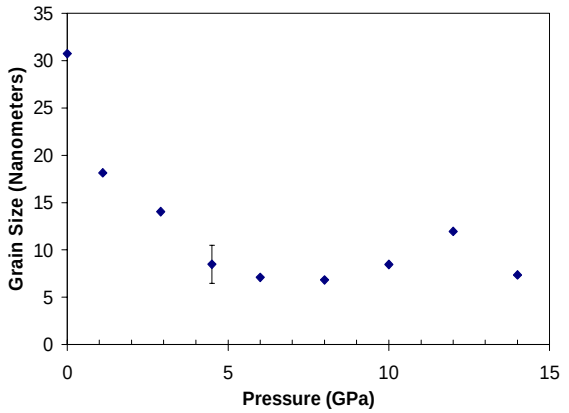

FIG. 2. Measured grain size of MgO sample at different pressures. The average experimental uncertainty is presented by the bar on the graph.

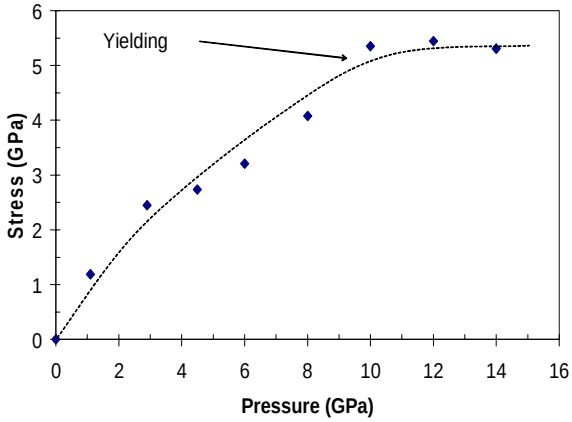

FIG. 3. Measured stress in the MgO sample as a function of pressure.

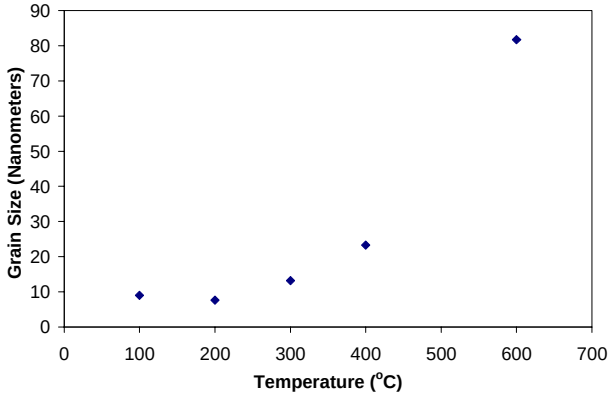

FIG. 4. Change in grain size of MgO sample during heating at 14 GPa.

linearly with the loading and yields when 5 Gpa is approached. This yield strength is significantly higher than the previously measured yield strength of the MgO powder sample with an average grain size in microns.

Upon heating at 14 GPa, the grain size starts increasing gradually (Fig. 4). At 600°C, the grain growth becomes significant, while the strength of the sample drops as a result of thermal relaxation.

Yield strength of MgO nanocrystals is measured for the first time using x-ray diffraction technique. A significant enhancement in yield strength is observed due to the nano-size crystals.

Acknowledgments

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