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The strength of moissanite

JIANZHONG ZHANG,[1,*] LIPING WANG,[1] DONALD J. WEIDNER,[1] TAKEYUKI UCHIDA,[2] AND JI-AN XU[3]

[1] Center for High-Pressure Research and Department of Geosciences, State University of New York at Stony Brook, Stony Brook, New York 11794, U.S.A.
[2] Consortium for Advanced Radiation Sources, University of Chicago, 5640 South Ellis Avenue, Chicago, Illinois 60637, U.S.A.
[3] The Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Road, N.W., Washington, D.C. 20015, U.S.A.

ABSTRACT

The yield strength of moissanite was investigated at pressures up to 18.3 GPa and temperatures up to 1200 °C by analyzing the peak shapes of diffraction lines from a powder sample. At room temperature, the moissanite crystal behaves elastically with increasing pressure up to 13.7 GPa. At higher pressures applied, the sample is yielded; the yield strength of moissanite is determined to be 13.6 GPa. Upon heating at 18.3 GPa, significant stress relaxation is observed at temperatures above 400 °C, and the yield strength of moissanite decreases rapidly from 12.8 GPa at 400 °C to 4.2 GPa at 1200 °C. Such behavior will place severe limitations on the use of moissanite as an anvil material when external heating is desired for high pressure and temperature experiments.

INTRODUCTION

Moissanite, a hexagonal silicon carbide compound, has recently been demonstrated to be, in many aspects, complementary to diamond, thus providing a promising window for high-pressure experiments (Xu and Mao 2000). Diamond, moreover, has limited availability and very high cost, which restricts high-pressure samples to microscopic volumes (10^{-13} to 10^{-16} m^3). Large, gem-quality, single-crystals of moissanite have recently become available; a scaled up diamond anvil cell (DAC) design with such large moissanite anvils will be suitable for compressing millimeter-sized samples to 50 GPa and will allow sample volumes 1000 times greater than those allowed in a typical DAC. A significant increase in the sample volume makes possible additional types of analysis, such as neutron diffraction, neutron scattering, inelastic X-ray spectroscopy, and ultrasonic interferometry. Moissanite is thermally stable up to at least 1127 °C when heated in air (Xu and Mao 2000), whereas diamond shows surface oxidation above 627 °C and burns above 847 °C (Fei and Mao 1994). In this regard, the moissanite anvils are believed to be particularly useful for high pressure-temperature experiments with resistive heating.

To evaluate the applications of moissanite anvils to high pressure-temperature research, one requires knowledge of the strength of moissanite, which is one of the fundamental properties that control the resistance to plastic deformation. In particular, the temperature dependence of the yield strength will define limitations on industrial applications of moissanite, if high temperature condition is desired, and on its use as anvil material for high-pressure experiments with external heating. Here we report results of stress measurement on moissanite at high pressure and temperature.

EXPERIMENTAL METHOD

Analysis of peak width is a common technique used to determine stress in metals and alloys (e.g., Westwood et al. 1995). In this study, we use the principles outlined by Weidner et al. (1994a) and Weidner (1998) to obtain information on stress and strength in powdered samples from X-ray diffraction signals. Following this method, deviatoric stress is introduced by compression of a powder sample and owes its origin to local stress concentrations that are necessary to accommodate the grain to grain contact. The effect of this microscopic deviatoric stress field is the broadening of diffraction lines, and the amount of line broadening is an indicator of the distribution of longitudinal elastic strain distribution parallel to the diffraction vector (Weidner et al. 1994a). The width of the diffraction lines is a convolution of the instrument response, sample response function, and the longitudinal elastic strain parallel to the diffraction vector. By assuming that the ambient diffraction data include the first two of these, we can calculate the full-width-half-maximum differential strain for Gaussian distribution at elevated pressure and temperature, which is given by

$$\varepsilon = (1/E)[W_o(E)^2 - W_i(E)^2]^{1/2} \quad (1)$$

where E is the X-ray photon energy, W_o the observed peak width at a given experimental condition, and W_i the instrumen-

* E-mail: zhang@sbmp06.ess.sunysb.edu

tal contribution. By multiplying the differential strain by an appropriate aggregate Young's modulus, one can convert the strain to stress, which is controlled by the strength of a material.

The moissanite sample (α-SiC 6H) studied was the same one used in Xu and Mao (2000). The strain measurements were performed on the powder sample using a DIA-type cubic anvil apparatus (Weidner et al. 1992) and a newly developed "T-Cup" high pressure system (Vaughan et al. 1998). An energy-dispersive X-ray method was employed using white radiation from the superconducting wiggler magnet at beamline X17B of the National Synchrotron Light Source and from the bending magnet at beamline 13-BM-D of the Advanced Photon Source. The incident X-ray beam was collimated to dimensions of 100×200 μm, and diffracted X-rays were collected with a solid-state Ge detector at fixed angles of 2θ, 6.4482°, and 5.6136° for the DIA and T-cup experiments, respectively.

In both experiments, a mixture of amorphous boron and epoxy resin was used as the pressure-transmitting medium and NaCl as an internal pressure standard. Amorphous carbon and Re were used as furnace materials in the DIA and T-cup experiments, respectively. Pressures were calculated from Decker's equation of state for NaCl (Decker 1971), and temperatures were measured by a W/Re25%–W/Re3% thermocouple that was positioned at the center of the furnace and was in direct contact with the sample and NaCl layers. X-ray diffraction patterns were typically collected in close proximity to the thermocouple junction for both moissanite and NaCl. No correction was applied for the effect of pressure on the thermocouple emf.

RESULTS AND DISCUSSION

At ambient conditions, the moissanite sample studied has a unit-cell volume of 124.65(4) $Å^3$ or an X-ray density of 3.213 g/cm^3. Because of a "blow-out" during the DIA experiment, only room-temperature data were collected for moissanite up to 6.7 GPa. In the T-Cup experiment, the sample was first compressed to 18.3 GPa at room temperature and then heated to 1200 °C at steps of 200 °C; no phase transformation was observed under these conditions. Figure 1 illustrates three diffraction peaks, (101), (102), and (103), at selected conditions along this experimental path. During the compression portion of the cycle the diffraction lines broaden asymmetrically up to 11.8 GPa, with the larger *d* spacing side of the peak remaining unchanged (Fig. 1a). This configuration indicates that in the moissanite aggregate, some of the grains do not support any of the applied stress. Therefore, the pressure is being supported by a subset of the moissanite grains and the supported stress is less than the yield strength of moissanite. This behavior is similar to what has been observed for diamond up to 10 GPa (Weidner et al. 1994b). Upon further compression, both sides of the diffraction peaks move to smaller *d* values (Fig. 1b), indicating the effect of compression on all of the moissanite grains. The peak width, however, is unchanged in the pressure range of 13.7–18.3 GPa.

Strictly speaking, Equation 1 can only be applied to a situation where the contribution of the grain size of the sample to the peak width broadening, W_s, can be ignored (Weidner et al. 1994a; Weidner 1998). As described by Gerward et al. (1976), a general form of Equation 1 is given by

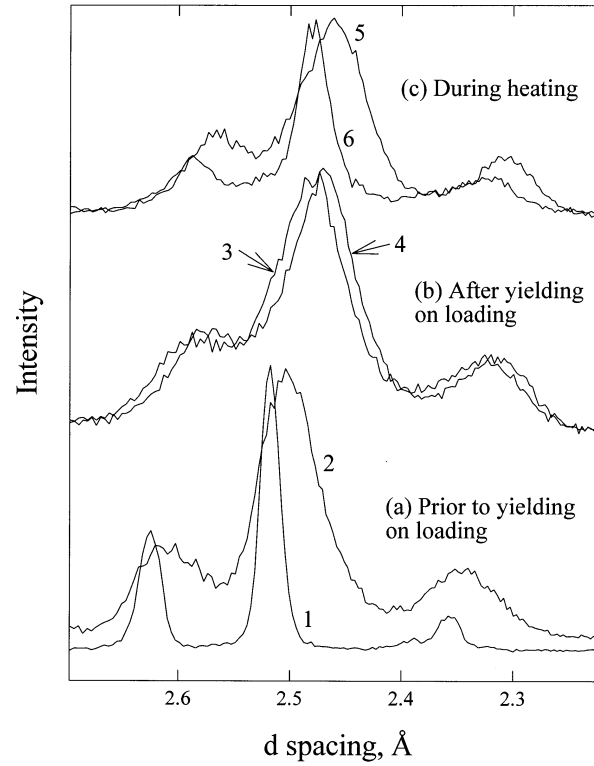

FIGURE 1. Diffraction peaks (from left to right), (101), (102), and (103), of moissanite at selected pressure and temperature conditions. Experimental conditions of the indicated patterns: 1 = ambient conditions; 2 = 10.3 GPa; 3 = 13.7 GPa; 4 = 17.5 GPa; 5 = 400 °C/18.4 GPa; 6 = 1200 °C/16.7 GPa. The counting time for each diffraction pattern is approximately 10 minutes.

$$W_o^2 - W_i^2 = W_s^2 + (\varepsilon E)^2 \quad (2)$$

To demonstrate the effect of grain size, the left-hand side of Equation 2 is plotted against energy squared for several diffraction peaks from the moissanite sample at 13.7 GPa and room temperature (Fig. 2). It is evident that the data can be fitted by a straight line with its intercept near zero at zero energy. The observed peak broadening (Fig. 1) is thus a result of strain, with $\varepsilon = 3.02(8) \times 10^{-2}$; it cannot be attributed to the sample grain size or to grain size reduction on loading.

Figure 3 shows the differential strain determined using Equation 1 and the (102) and (110) diffraction lines as a function of applied pressure at room temperature and as a function of temperature at constant ram load (corresponding to 17–18 GPa). The similarity between the strain data from the DIA and T-Cup experiments suggests that it is the material properties that have been measured, not the characteristics of the sample assembly. The linear dependence of the strain with pressure up to 13.7 GPa indicates that the loading process is elastic. Above this pressure, the strain saturates and remains approximately constant with further loading to 18.3 GPa. This indicates that in this range of applied pressure deviatoric stress exceeds the yield strength of moissanite and it has begun to deform. To convert strain to stress, we use an aggregate Young's modulus, 447 GPa,

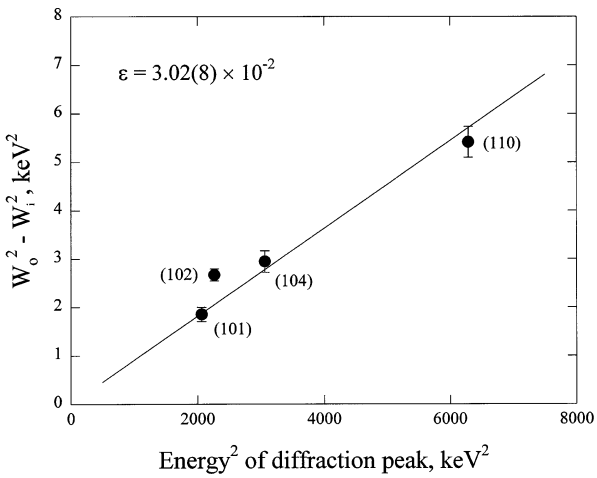

FIGURE 2. Energy-dependent peak broadening for moissanite at 13.7 GPa and room temperature. Slope of the straight line reflects the strain contribution to broadening, and the intercept reflects the grain size broadening. The plotted error bars refer to the propagated errors in the peak width determinations at ambient and experimental conditions.

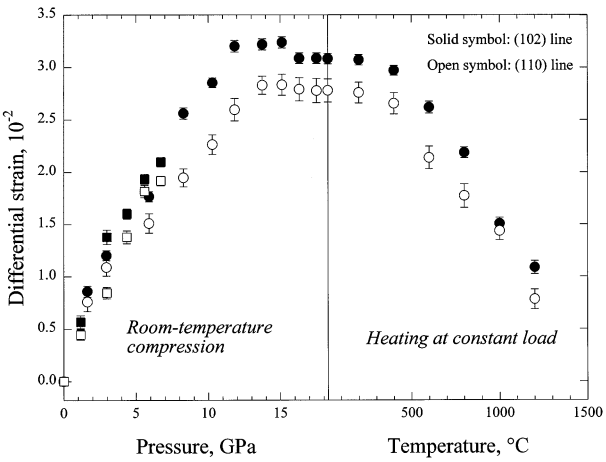

FIGURE 3. Differential strain determined from the broadening of the (102) and (110) diffraction peaks of moissanite at various pressure and temperature conditions. Square and circle symbols correspond to the data from the DIA and T-Cup experiments, respectively. The plotted error bars reflect the propagated errors in the peak width determinations for the (102) and (110) diffraction lines. Note that at 13.7 GPa the average strain determined from these two peaks is the same as that obtained in Figure 2.

for moissanite, which was calculated from the bulk (220 GPa) and shear (192.5 GPa) moduli determined for polycrystalline α-SiC (6H) (Feng et al. 1996). Since the sample has already been yielded at 13.7 GPa, the maximum differential stress that can be supported by the moissanite grains represents the yield strength of moissanite, which is 13.6 GPa at ambient temperature or equivalent to the maximum shear stress of 6.8 GPa. The errors in the strength measurements of this study are typically 0.5 GPa when uncertainties in strain (Fig. 3) are taken into account. For comparison, the maximum shear stress that can be supported by moissanite in the shock state was found to be 7 GPa at an applied pressure of 21 GPa (Feng et al. 1998).

As temperature is increased at 18.3 GPa, the shape of the diffraction peak is maintained up to 400 °C (Fig. 1c). In this temperature region, however, there is no clear evidence of thermally induced stress relaxation (Fig. 3). Above this temperature, the diffraction peaks begin to narrow (Fig. 1c), and the strain diminishes with further heating to 1200 °C (Fig. 3). Within a time scale of 20–25 min., no time-dependent stress relaxation was observed at 600 and 1200 °C. In Figure 4, we show the yield strength of moissanite as a function of temperature at 18 GPa. The yield strength of moissanite decreases rapidly with temperature from 12.8 GPa at 400 °C to 4.2 GPa at 1200 °C. For comparison, the yield strength of diamond (Fig. 4) was estimated to be 15 GPa at 1200 °C and 6 GPa at 1550 °C (Weidner et al. 1994b). As expected, moissanite is much weaker than diamond, even though the rate of thermally induced weakening in diamond is substantially greater than that in moissanite.

These results have implications for the development of the next generation of large-volume, high-pressure apparatuses with moissanite as the anvil material (Xu and Mao 2000). As illustrated in Figure 4, the strength of moissanite is highly compromised at temperatures above 400 °C. Above 1000 °C, it becomes even weaker than tungsten carbide at ambient temperature (~6 GPa; Ashby and Jones 1993). Such behavior will place severe limitations on the use of moissanite as an anvil material when external heating is desired for high pressure and temperature experiments.

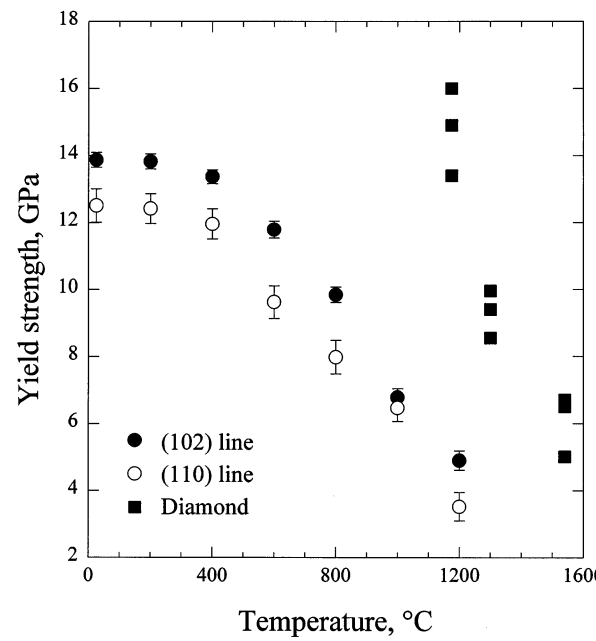

FIGURE 4. Yield strength of moissanite (circles) as a function of temperature, calculated from the multiplication of the strain-broadening of the indicated peaks by Young's modulus for moissanite, 447 GPa. The strength data for diamond are from Weidner et al. (1994b). In text, we use the average values measured for different diffraction peaks to represent the yield strength at a given temperature.

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