

X-ray diffraction and Raman studies of beryllium: Static and elastic properties at high pressures

W. J. Evans, M. J. Lipp, H. Cynn, and C. S. Yoo

H-Division, Physics and Advanced Technologies, Lawrence Livermore National Laboratory, Livermore, California 94551, USA

M. Somayazulu and D. Häusermann

HPCAT, Argonne National Laboratory, Carnegie Institution of Washington, Advanced Photon Source, Building 434E, 9700 South Cass Avenue, Argonne, Illinois 60439, USA

G. Shen and V. Prakapenka

GSECARS, CARS-The University of Chicago, Advanced Photon Source, Building 434A, 9700 S. Cass Ave., Argonne, Illinois 60439, USA

(Received 29 May 2005; published 26 September 2005)

We report combined x-ray and Raman studies of beryllium in helium and argon pressure media at pressures approaching 200 GPa. Our results are generally consistent with recent studies confirming the stability of the hexagonal close-packed phase to the highest pressures. However, the quasi-hydrostatic conditions of our studies lead to a stiffer equation of state ($K_0=109.88$, $K'_0=3.59$) and a gradual approach toward a more ideal c/a ratio of 1.60 at 180 GPa. Combining our Raman and equation of state data, we are able to evaluate the pressure dependence of the elastic shear modulus ($C_{44}=109.3$, $C'_{44}=1.959$). We discuss the comparison of our results with measurements using ultrasonic and dynamic techniques.

DOI: [10.1103/PhysRevB.72.094113](https://doi.org/10.1103/PhysRevB.72.094113)

PACS number(s): 62.50.+p, 61.66.Bi, 64.30.+t, 63.20.-e

I. INTRODUCTION

Beryllium is a unique metal with unusual properties of technological and scientific importance. Its physical properties are useful to the nuclear power industry as a neutron reflector/moderator and as a stiff lightweight structural element for aerospace structures. Further, beryllium exhibits an unusually high Debye temperature that leads to a large specific conductance and has thus been identified as a “hyperconductor” with favorable properties for efficient transmission of electrical power.¹ This combination of unique properties and unusual behavior contribute to the characterization of beryllium as an “anomalous” metal. Scientifically beryllium has been the subject of a great deal of interest because of its simple atomic configuration and anomalous behavior. A simple atom with only two valence electrons (four total) would appear to be amenable to precise theoretical and *ab initio* modeling approaches. Contrary to this supposition, beryllium has been a difficult system to model and accurate theoretical predictions of its properties at high pressures have been elusive.²⁻⁵ To address this broad interest, we have undertaken experimental studies of beryllium under high-pressure conditions. Experimental studies of beryllium at high pressures measure the density dependence of fundamental properties, which will enable new applications and advance the basic scientific understanding of this material.

Beryllium at high pressure has been the subject of several experimental⁶⁻¹⁹ and theoretical studies.^{2-5,20-22} At ambient conditions beryllium is a metal with a hexagonal close packed (hcp) crystal structure (α phase) and a c/a ratio of 1.56,²³ far from the ideal value of 1.633. This nonideal behavior is ascribed to the highly anisotropic bonding properties.^{3,5} At ambient pressure and high temperature beryllium transforms to a body centered cubic (bcc) crystal structure (β phase) at 1523 K, melts at 1551 K, and finally

boils at ~ 3243 K.²⁴ At elevated pressure (up to 6 GPa) and high temperature, the α - β phase line has been observed to decrease with increasing pressure, with a negative slope of 45 K/GPa.⁸ These data are summarized in the phase diagram shown in Fig. 1.

The α - β phase line (hcp-bcc) has been the source of continuing interest and controversy.^{6,9,17} At ambient pressure, high-temperature experimental x-ray diffraction studies identified this hcp-bcc transition and measured an unusually large 4% decrease in specific volume.²⁵ At high pressures, the phase line was determined indirectly by monitoring the resistance of a beryllium sample in a belt-type large volume press.⁸ A change in the resistance-versus-temperature slope was observed and used to identify the α - β phase line. Linearly extrapolating these data to room temperature, the phase line would be expected to cross 21 GPa at 300 K. It should

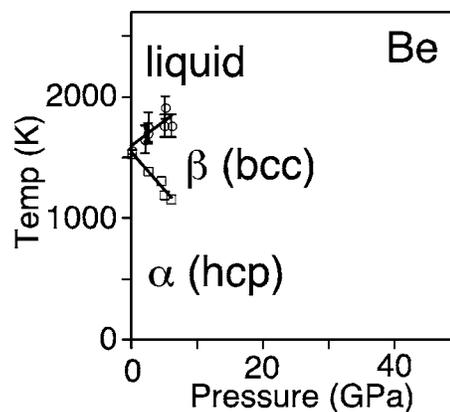


FIG. 1. Phase diagram of beryllium. High pressure data of Francois and Contre (Ref. 8) establishing the hcp, bcc, and liquid phase lines are shown.

be noted that there is some controversy regarding this observation.⁶ Nevertheless, this negative slope stimulated several experimental and theoretical efforts to locate the continuation of this α - β phase line at room temperature. While several high-pressure electrical conductivity studies observed changes interpreted as the α - β transition,^{17,26} recent x-ray diffraction studies have found no such transitions.^{10,16} Theoretical efforts have found beryllium to be a challenging system, with predictions of the α - β phase line varying from 20 to 200 GPa.^{4,5,21,27} Thus previous studies have reported widely varying results.

Beryllium is a material with unique properties presenting both challenges and unique opportunities for experimental studies. As a low- Z element, beryllium has a very poor x-ray scattering efficiency, making diffraction measurements challenging. However, the light mass and hcp structure of beryllium lead to a single relatively high frequency Raman-active phonon mode (doubly degenerate E_{2g}) that is suitable for Raman scattering measurements.

Recent studies of beryllium have addressed some of the controversial aspects of earlier work,^{10,16} but several questions remain. X-ray synchrotron studies of beryllium have established the stability of the hcp structure at room temperature to pressures approaching 200 GPa.¹⁰ However, the experiments were performed without a hydrostatic pressure medium, so some question remains regarding the accuracy of the lattice constants. Most importantly, the high stability of the hcp phase is in sharp contrast with the results of earlier low-pressure experiments^{8,17,26} and theoretical predictions^{4,5,21} and warrants confirmation. There has been one previous Raman spectroscopy study of beryllium at high pressure,¹² up to 30 GPa. In addition to static high-pressure studies of beryllium, there have been a few notable dynamic shock^{11,19,28,29} and isentropic compression experiments,^{14,15,18} that complement static high pressure measurements and lead to the possibility of constructing a complete p - V - T equation of state.

In this report we present the results of studies using high-performance synchrotron sources to measure the crystal structure, lattice constants, and equation of state of beryllium to a pressure approaching 200 GPa (or 2.0 Mbar). Complementing the x-ray studies, we have measured the Raman spectrum of beryllium to pressures approaching 100 GPa. Combining both of these data, we evaluate the pressure dependence of the elastic shear modulus C_{44} . Finally, we discuss the implications of our work on the understanding of the properties of beryllium at high pressures.

II. EXPERIMENTAL PROCEDURE

The data presented in this paper are the result of several x-ray diffraction and Raman spectroscopy experimental runs on beryllium using modern diamond anvil cell (DAC) techniques. We used Livermore-designed DACs of a modified Mao-Bell type and membrane-driven DACs. The anvils were 300 μm flat diamonds and 300 μm culet/100 μm flat single-beveled diamonds for pressures below and above 50 GPa, respectively. Rhenium gaskets were preindented to thicknesses of 20–40 μm and drilled with sample chamber

holes of 50–150 μm . Beryllium samples were prepared by acid etching and rinsing a polycrystalline beryllium foil (Brush-Wellman, electrorefined 99.8% purity) to remove oxides and contaminants and carefully cutting a 20–50 μm piece from the foil. The beryllium piece was loaded into the gasket hole along with a few micron-sized particles of gold (ruby) for *in situ* pressure determination during the x-ray diffraction (Raman spectroscopy) run. We used hydrostatic pressure media in all of the experiments. In the case of x-ray diffraction, we used cryogenic techniques to load liquid helium, thereby minimizing diffraction signals from the pressure medium. Liquid argon was loaded cryogenically and served as the pressure medium in the cells designated for Raman spectroscopy.

X-ray diffraction was performed at both GSECARS and HPCAT beamlines of the Advanced Photon Source (Argonne, IL). X-ray spot sizes were ~ 20 μm and energies of 22 and 37 keV were used. The diffracted x-ray signal was detected using an image plate using exposure times of 5 min. The pressure was determined *in situ* using the equation-of-state of the gold pressure marker.³⁰ The aperture in the diamond anvil cell limited the 2θ -scattering angle to $\sim 25^\circ$. The x-ray diffraction images consisted of uniform rings. Several diffraction peaks were observed below 100 GPa, including the (100), (002), (101), (102), (110), and (103). Above 100 GPa, the physical dimensions of the aperture in the DAC and the x-ray energy limited observed diffraction lines to the (100) and (101). Although these two lines are insufficient to make a structural determination, continuity with more complete spectra supports these peak identifications. Representative diffraction spectra are shown in Fig. 2. X-ray diffraction from the beryllium and gold pressure marker were measured simultaneously by selecting a spot on the sample where both materials were present. This approach minimized any possible systematic errors due to pressure gradients and ensured accurate *in situ* pressure measurements. Pressure determinations based on the accuracy of the gold diffraction peak determination were accurate to better than 0.5 GPa. The lattice constants a and c of beryllium were measured to accuracies of better than 0.02% and 0.1%, respectively.

Raman spectroscopy was performed using the 488 nm laser line of an argon ion laser. The laser was focused to a spot size of 15 μm with an incident power level of less than 30 mW at the sample. The Raman scattered light was collected at an angle of $\sim 30^\circ$ with respect to the incident laser beam. The Raman signal was spatially filtered and analyzed using a holographic notch filter, a 0.3 m spectrograph, and a liquid-nitrogen-cooled charge-coupled device (CCD) detector with an instrumental resolution of 0.24 cm^{-1} . Typical exposure times were 5 min, gradually increasing to 30 min at our highest pressures near 100 GPa. The Raman phonon mode of beryllium was clearly evident, though more than 5×10^{-3} weaker than the diamond Raman signal. This weak signal is not inconsistent with the findings of previous polarized Raman studies of single crystals at ambient pressure. We observed no signal in the regime of the beryllium oxide phonon,³¹ indicating a relatively pure sample with minimal oxide contamination. Pressure was determined *in situ* using the ruby fluorescence technique,³² with an accuracy of 0.5 GPa. Raman peaks were fitted and peak positions were de-

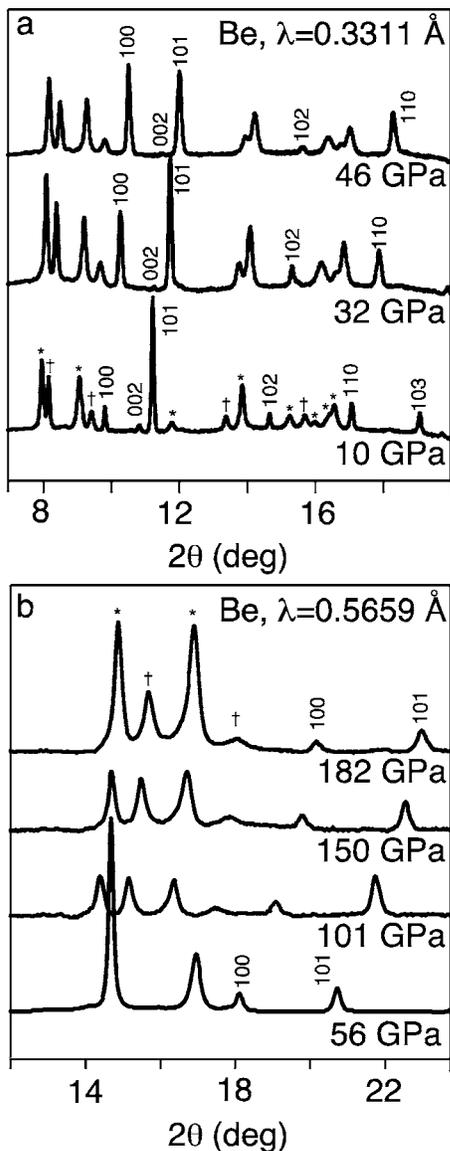


FIG. 2. Representative x-ray diffraction patterns over the pressure range covered in this report. (a) and (b) are at x-ray photon wavelengths of 0.3311 and 0.5659 Å, respectively. Pressures are indicated adjacent to trace. Peaks due to the rhenium gasket and gold pressure marker are marked with an asterisk (*) and dagger (†), respectively.

terminated with typical accuracies of 0.2 cm^{-1} . At the pressures above 60 GPa, the weakening signal strength led to a gradual decrease in accuracy to 1.0 cm^{-1} . The linewidth [full width at half maximum (FWHM)] of the Raman mode increased approximately linearly with pressure from 7.97 cm^{-1} at ambient pressure to 31.6 cm^{-1} at 82 GPa. As with the x-ray diffraction, the pressure and Raman were collected from the same location without any repositioning to ensure that pressure gradients did not introduce systematic errors in the correlation of pressure to Raman spectrum. There was no observable pressure gradient across the sample chamber to within the accuracy of our pressure measurement. The Raman experiments ended not because of diamond anvil failure, but a gradual decrease in the Raman signal strength,

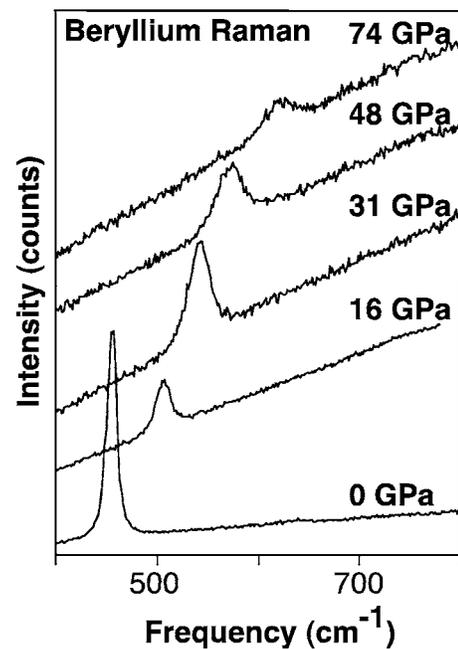


FIG. 3. Representative Raman spectra spanning the pressure range covered in this report. Pressure is indicated adjacent to spectra. Spectra are scaled and shifted for clarity.

probably due to the increasingly strong diamond background. A sampling of the collected Raman spectra is shown in Fig. 3.

III. ANALYSIS AND RESULTS

We present now the results of several experimental runs measuring x-ray diffraction and Raman spectra of beryllium under pressure. We were able to achieve pressures approaching 200 and 100 GPa for x-ray diffraction and Raman spectroscopy, respectively. Using a previously developed theoretical framework, we use these data to calculate the pressure dependence of the elastic shear modulus of beryllium.

Beryllium was pressurized to a maximum pressure of 182 GPa. Consistent with previous studies,¹⁰ beryllium remains in the hcp structure at room temperature and we find no evidence of any structural phase transitions. In Fig. 4 we present a graph of the isothermal equation of state at room temperature. For comparison, data from other works are included. We fit our data to a third-order Birch-Murnaghan equation, yielding parameters of $109.88(1.05) \text{ GPa}$ and $3.584(0.027)$ for the bulk modulus and its pressure derivative, respectively. Figure 4 shows the pressure dependence of the c/a ratio, which is initially flat, but above 60 GPa increases monotonically. Based on the accuracies stated above, the accuracy of the equation of state (EOS) and c/a ratio is dominated by the accuracy of our measurement of c and is thus $\sim 0.1\%$.

Our Raman studies extend up to 80 GPa, again showing no evidence of a phase transition and are in good agreement with the previous work of Olijnyk and Jephcoat at lower pressures.¹² We measured the Raman phonon energy to be 453.7 cm^{-1} at ambient pressure. This differs somewhat with

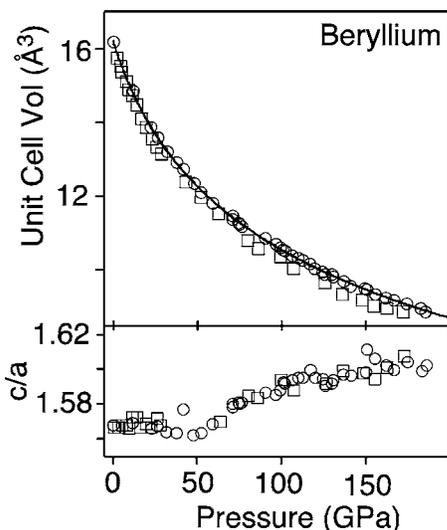


FIG. 4. Equation of state and c/a ratio of beryllium measured in this work (open circles). For comparison, the measurements of Nakano *et al.* (Ref. 10) (open squares) are shown. Upper panel shows unit cell volume as a function of pressure. Lower panel shows the change in the c/a ratio with pressure.

the measurement of Olijnyk and Jephcoat (457 cm^{-1}),¹² but is consistent with the studies of Feldman *et al.*³³ (455 cm^{-1}). It is important to note that Olijnyk and Jephcoat used the 514.5 nm laser line for Raman excitation, while our studies and those of Feldman *et al.* used the 488 nm line. This Raman energy dependence on excitation wavelength may be attributed to a strong phonon dispersion/probed wave vector effect, as noted by Ponosov *et al.* in the case of Osmium.^{34,35} Figure 5 shows the pressure dependence of the Raman phonon line center. The pressure dependence is approximately linear in pressure with a slight decrease in slope with increasing pressure. We fit the data to a second-order polynomial in pressure (units of GPa) with coefficients 459(2.1), 2.806(0.113), and $-0.011(0.001)$.

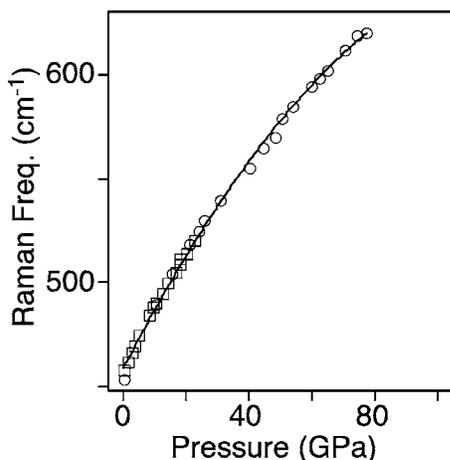


FIG. 5. Pressure dependence of the Raman shift of the TO phonon in beryllium. Circles are this work and squares are the work of Olijnyk and Jephcoat (Ref. 12). The straight line is a second-order polynomial fit to our data, $E \text{ (in cm}^{-1}\text{)} = 459 + 2.806 P \text{ (in GPa)} - 0.011 P^2$.

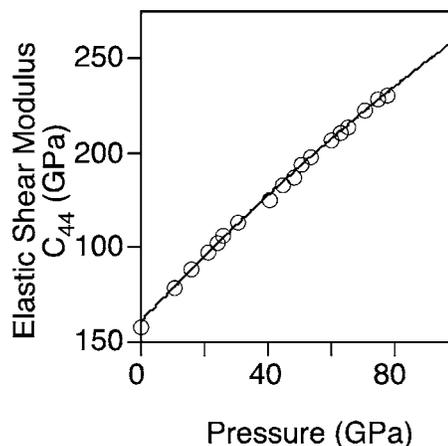


FIG. 6. Pressure dependence of the elastic shear modulus of beryllium. Circles are calculations using our data, and the line is a second-order polynomial fit, $C_{44} \text{ (in GPa)} = 110.6 + 1.784 P \text{ (in GPa)} - 0.0028 P^2$.

Using the collected data, we have calculated the elastic shear modulus of beryllium. The Raman phonon mode being measured represents a collective excitation where adjacent hexagonal planes of atoms oscillate against each other. Thus it is reasonable to expect that the Raman phonon reflects the behavior of the elastic shear modulus C_{44} . An expression for the elastic shear modulus has been derived for the hcp structure with the assumption of isotropic interaction potentials.^{12,36–40} The expression describing this relationship, as given by Olijnyk and Jephcoat¹² is

$$\nu_{TO}(k=0) = \sqrt{\frac{\sqrt{3}a^2 C_{44}}{\pi^2 mc}}.$$

Using the result of our EOS fit to the beryllium p - V data, we apply this expression and calculate the elastic shear modulus C_{44} . The results of this calculation are shown in Fig. 6. Propagating the errors in the parameters, the accuracy of our determination of C_{44} is approximately 1%. Our results are in good agreement with the work of Olijnyk and Jephcoat¹² and extend the experimentally measured range of the dependence to pressures approaching 100 GPa. A quadratic fit to the data points versus pressure yields the parameters 110.6(1.0), 1.784 (0.056), and -0.0028 (0.0007) for the y intercept, slope, and second derivative, respectively. The small second derivative demonstrates that the relation is generally linear over this pressure range.

IV. DISCUSSION

Our x-ray diffraction studies yield an isothermal EOS that differs noticeably from previous studies. Our measured EOS is substantially stiffer than the EOS of Nakano *et al.*¹⁰ This is clearly evident in Fig. 4, amounting to a 2–4% difference in volume at pressures above 100 GPa. The cause of this difference is not clear, but could possibly be due to systematic effects in determining the pressure in a nonhydrostatic sample with a pressure gradient. We tentatively ascribe the difference to the use of a hydrostatic medium, helium,

TABLE I. Comparison of bulk modulus and its derivative for static and dynamic measurements.

Technique	K_0	K'_0
DAC ^a	109.88 (1.05)	3.59 (0.03)
DAC ^b	97.2 (2.5)	3.61 (0.007)
DAC ^c	106.5	3.541
Shock ^d	114.97	3.55

^aThis work.^bReference 10.^cReference 16.^dReference 28.

whereas the previous studies used no medium. We note that our results agree quite well with the work of Velisavljevic *et al.*,¹⁶ where a copper pressure-calibrant/medium was used up to a pressure of 66 GPa. More generally our bulk modulus and its derivative are in reasonable agreement with dynamic measurements shown in Table I (the bulk modulus for the shock measurement was determined by fitting a Birch-Murnaghan function to the $T=0$ isotherm that had been deduced from the shock data²⁸). The static isothermal pV data we present here may be combined with a detailed analysis of recent dynamic measurements^{11,15,18,19} to construct an experimentally validated complete pVT EOS.

An interesting finding of our work is the increase of the c/a ratio from 1.56 at ambient pressure to 1.60 at 180 GPa. The increase in the c/a ratio occurs at pressures above 50 GPa, just beyond the range of previous work that observed no significant variation.¹⁶ The deviation of the c/a ratio of beryllium at ambient pressure is ascribed to anisotropic bonding, namely, a strongly covalent bond character, with a component aligned along the c axis.⁵ The gradual increase in the c/a ratio observed in our studies suggests an increasingly isotropic interatomic potential. This change is important because it serves to justify our use of the model described above for the elastic shear modulus of beryllium. In particular, the model was developed assuming an isotropic force potential. Thus, because our lattice constant measurements imply an increasingly isotropic potential, we expect our evaluation of C_{44} to be increasingly valid at higher pressures. For the purpose of validating theoretical modeling efforts, one would expect credible approaches to reproduce not only the pV data but also the change in the c/a ratio. We further note that recent studies suggest that such an abrupt shift in the c/a dependence may be the result of a Lifshitz electronic transition.⁴¹ Occelli *et al.*⁴¹ identified a subtle discontinuity in the slope of the c/a pressure dependence of osmium and associate this with an electronic anomaly. Although there are conflicting measurements⁴² of osmium regarding the presence of this discontinuity, in the case of beryllium we find an abrupt clearly identifiable change in slope at ~ 50 GPa. Within the context of the proposed Lifshitz transition, our measurements of beryllium present a compelling case for further theoretical and experimental study.

Our evaluation of C_{44} differs markedly from ambient pressure ultrasonic measurements,^{43,44} but is consistent with the work of Olijnyk and Jephcoat,¹² as shown in Table II. At

TABLE II. Comparison of C_{44} evaluation.

Technique	C_{44} (GPa)	C'_{44}
DAC ^a	110.6 (1.0)	1.78(0.06)
DAC ^b	110	1.65
Ultrasonic ^c	154.9	
Ultrasonic ^d	170.6	2.55

^aThis work.^bReference 12.^cReference 43.^dReference 44.

ambient pressure, ultrasonic determinations are as much as 54% larger than the value we report. Similarly the pressure derivatives are also 43% larger in the case of ultrasonic measurements. Although no accuracy is reported for the ultrasonic work, based on the technique, we expect the measurements to be good to a few percent. Unfortunately ultrasonic measurements become increasingly challenging under pressure and are unheard of at the ultrahigh pressures achieved in our work. The anisotropic bonding of beryllium at low pressures is a possible explanation for the observed deviation between our evaluation and the results of ultrasonic measurements. Namely, the model we have used is not entirely appropriate for the low-pressure anisotropic bonding, however it will become increasingly valid as the pressure and thus the c/a ratio approaches a value consistent with an isotropic potential. If one assumes that the accuracy of our measurements scales with the relative deviation from the ideal c/a ratio, we speculate that at 80 GPa, our evaluation is within 20% of the actual value. This is an admittedly crude approximation, but a reasonable estimate in the absence of a more sophisticated model. Thus despite the limitations of the model, we believe our evaluation of C_{44} to be increasingly accurate at higher pressures.

V. CONCLUSION

In summary, we have measured the room temperature lattice constants and Raman phonon of beryllium under hydrostatic conditions up to pressures of 180 and 80 GPa, respectively. We determine the bulk modulus and its derivative to be 109.88 and 3.584. The c/a ratio increases with pressure achieving 1.60 at 180 GPa. The Raman phonon shifts linearly with pressure, fitting to a line with an initial value of 459 cm^{-1} and a slope of $2.806 \text{ cm}^{-1}/\text{GPa}$. Finally we used our data to evaluate the elastic shear modulus, which fits to a line beginning at 110.6 GPa and a slope of 1.784. Although we find qualitative agreement with previous studies, our measured EOS is stiffer than nonhydrostatic studies. Our Raman studies increase the measured pressure range by more than a factor of two, and permit the evaluation of the elastic shear modulus to pressures approaching 100 GPa. We do not observe any phase transitions at room temperature. These data should be valuable in the modeling of beryllium under pressure and developing a complete pVT EOS model of this technologically important material.

ACKNOWLEDGMENTS

This work was performed under the auspices of the U.S. DOE by the University of California, LLNL under Contract No. W-7405-Eng-48. Work performed at HPCAT was supported by DOE-BES, DOE-NNSA (CDAC), NSF, DOD-TACOM, and the W.M. Keck Foundation and at GeoSoilEnviroCARS, by the NSF-Earth Sciences (EAR-0217473),

DOE-Geosciences (DE-FG02-94ER14466) and the State of Illinois. Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. W-31-109-ENG-38. The authors acknowledge use of the program FIT2D developed by A. Hammersley of ESRF. We thank Sam Weir for useful discussions.

-
- ¹F. M. Mueller, K. A. Johnson, W. J. Medina, H. D. Lewis, D. S. Phillips, M. F. Hundley, J. D. Thompson, Z. Fisk, L. A. Jacobson, C. J. Maggione, J. F. Smith, E. M. Honig, W. L. Gordon, J. E. Schirber, and R. Kossowsky, *Appl. Phys. Lett.* **57**, 240 (1990).
- ²M. Y. Chou, P. K. Lam, and M. L. Cohen, *Solid State Commun.* **42**, 861 (1982).
- ³M. Y. Chou, P. K. Lam, and M. L. Cohen, *Phys. Rev. B* **28**, 4179 (1983).
- ⁴P. K. Lam, M. Y. Chou, and M. L. Cohen, *J. Phys. C* **17**, 2065 (1984).
- ⁵A. K. McMahan, *AIP Conf. Proc.* **78**, 340 (1981).
- ⁶A. Abey, (Lawrence Livermore National Laboratory, Livermore, CA, 1984), p. 13.
- ⁷A. E. Abey and R. L. Reichlin, *Bull. Am. Phys. Soc.* **26**, 667 (1981).
- ⁸M. Francois and M. Contre, in *Conference Internationale sur la Metallurgie du Beryllium* (Universite de France, Paris, Grenoble, 1965).
- ⁹L. C. Ming and M. H. Manghni, *J. Phys. F: Met. Phys.* **14**, L1 (1984).
- ¹⁰K. Nakano, Y. Akahama, and H. Kawamura, *J. Phys.: Condens. Matter* **14**, 10569 (2002).
- ¹¹W. J. Nellis, J. A. Moriarty, A. C. Mitchell, and N. C. Holmes, *J. Appl. Phys.* **82**, 2225 (1997).
- ¹²H. Olijnyk and A. P. Jephcoat, *J. Phys.: Condens. Matter* **12**, 8913 (2000).
- ¹³R. L. Reichlin, *Rev. Sci. Instrum.* **54**, 1674 (1983).
- ¹⁴D. C. Swift, D. L. Paisley, G. A. Kyrala, and A. Hauer, *AIP Conf. Proc.* **620**, 1192 (2002).
- ¹⁵D. Swift, D. Paisley, and M. Knudson, *AIP Conf. Proc.* **706**, 119 (2004).
- ¹⁶N. Velisavljevic, G. N. Chesnut, Y. K. Vohra, S. T. Weir, V. Malba, and J. Akella, *Phys. Rev. B* **65**, 172107 (2002).
- ¹⁷V. Vijayakumar, B. K. Godwal, Y. K. Vohra, S. K. Sikka, and R. Chidambaram, *J. Phys. F: Met. Phys.* **14**, L65 (1984).
- ¹⁸D. B. Reisman, A. Toor, R. C. Cauble, C. A. Hall, J. R. Asay, M. D. Knudson, and M. D. Furnish, *J. Appl. Phys.* **89**, 1625 (2001).
- ¹⁹R. Cauble, T. S. Perry, D. R. Bach, K. S. Budil, B. A. Hammel, G. W. Collins, D. M. Gold, J. Dunn, P. Celliers, L. B. Da Silva, M. E. Foord, R. J. Wallace, R. E. Stewart, and N. C. Woolsey, *Phys. Rev. Lett.* **80**, 1248 (1998).
- ²⁰H. C. Graboske, R. Grover, and K. Long, *Bull. Am. Phys. Soc.* **24**, 724 (1979).
- ²¹B. Palanivel, R. S. Rao, B. K. Godwal, and S. K. Sikka, *J. Phys.: Condens. Matter* **12**, 8831 (2000).
- ²²D. A. Young, *Phase Diagrams of the Elements* (University of California Press, Berkeley, 1991).
- ²³J. Donohue, *The Structures of the Elements* (Wiley, New York, 1974).
- ²⁴J. Elmsley, *The Elements* (Oxford University Press, London, 1998).
- ²⁵A. J. Martin and A. Moore, *J. Less-Common Met.* **1**, 85 (1959).
- ²⁶A. R. Marder, *Science* **142**, 664 (1963).
- ²⁷J. C. Boettger, *Int. J. Quantum Chem.* **56**, 197 (1995).
- ²⁸R. G. McQueen, S. P. Marsh, J. W. Taylor, J. N. Fritz, and W. J. Carter, in *High-Velocity Impact Phenomena*, edited by R. Kin-slow (Academic Press, New York, 1970).
- ²⁹J. L. Wise, L. C. Chhabildas, and J. R. Asay, *AIP Conf. Proc.* **78**, 417 (1982).
- ³⁰O. L. Anderson, D. G. Isaak, and S. Yamamoto, *J. Appl. Phys.* **65**, 1534 (1989).
- ³¹A. P. Jephcoat, R. J. Hemley, H. K. Mao, R. E. Cohen, and M. J. Mehl, *Phys. Rev. B* **37**, 4727 (1988).
- ³²H. K. Mao, J. Xu, and P. M. Bell, *J. Geophys. Res.* **91**, 4673 (1986).
- ³³D. W. Feldman, J. H. Parker, Jr., and M. Ashkin, *Phys. Rev. Lett.* **21**, 607 (1968).
- ³⁴Y. S. Ponomov, G. A. Bolotin, C. Thomsen, and M. Cardona, *Phys. Status Solidi B* **208**, 257 (1998).
- ³⁵Y. S. Ponomov, I. Loa, V. E. Mogilenskikh, and K. Syassen, *Phys. Rev. B* **71**, 220301 (2005).
- ³⁶E. A. Metzbowyer, *Phys. Status Solidi* **25**, 403 (1968).
- ³⁷H. Olijnyk and A. P. Jephcoat, *Solid State Commun.* **115**, 335 (2000).
- ³⁸H. Olijnyk and A. P. Jephcoat, *High Press. Res.* **22**, 43 (2002).
- ³⁹H. Olijnyk and A. P. Jephcoat, *Metall. Mater. Trans. A* **33**, 743 (2002).
- ⁴⁰J. C. Upadhyaya, D. K. Sharma, D. Prakash, and S. C. Upadhyaya, *Can. J. Phys.* **72**, 61 (1994).
- ⁴¹F. Ocellini, D. L. Farber, J. Badro, C. M. Aracne, D. M. Teter, M. Hanfland, B. Canny, and B. Couzinet, *Phys. Rev. Lett.* **93**, 109901 (E) (2004).
- ⁴²T. Kenichi, *Phys. Rev. B* **70**, 012101 (2004).
- ⁴³W. D. Rowland and J. S. White, *J. Phys. F: Met. Phys.* **2**, 231 (1972).
- ⁴⁴D. J. Silversmith and B. L. Averbach, *Phys. Rev. B* **1**, 567 (1970).