COMPRES

Newsletter

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Project Report

Challenges in Pressure Calibration at High Temperatures

A correct pressure scale is fundamentally important for high-pressure research. It allows us to make comparisons of high-pressure results produced in different laboratories and by using different techniques and methods. In practice, pressures in a multi-anvil apparatus are calibrated by using known pressure fix points, whereas pressures in a diamond-anvil cell are measured using a ruby pressure scale. These secondary pressure scales were established through in-situ X-ray diffraction measurements of pressure standards such as NaCl, MgO, Au, W, Mo, Pt, Cu, Ag, and Pd. Such pressure determinations rely on the accuracy of *P-V-T* equations of state (EOS) of the pressure standards, which are primarily derived from shock compression and thermodynamic data.

IN THIS ISSUE:

The ruby fluorescence pressure gauge has been successfully used in diamond-anvil experiments for pressure determination at room temperature. The ruby gauge was calibrated by simultaneously measuring the shift of ruby R_1 luminescent line and specific volume of metal standards (Cu, Mo, Pd, and Ag) as a function of pressure. The established calibration curve based on equations of state of metal standards (Mao et al., 1986) has proven to be accurate, confirmed by direct measurements of pressure by combining Brillouin scattering and X-ray diffraction techniques (Zha et al., 2000). The use of the ruby gauge has made it possible to compare the existing room-temperature high-pressure data accumulated over the last several decades.

Accurate determination of pressure at high temperature is more difficult because of large uncertainty in calculating the thermal pressure. Gold (Au), platinum (Pt), MgO, and NaCl have been extensively used as internal pressure standards in

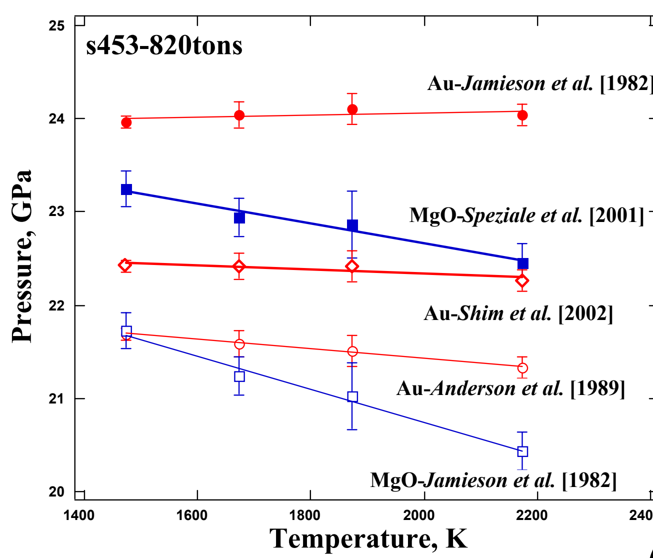

Figure 1 Calculated pressures using MgO and Au pressure scales at high temperatures. Solid circles, open diamonds, and open circles represent pressures calculated from Au scales by Jamieson et al. (1982), Shim et al. (2002), and Anderson et al. (1989), respectively. Solid and open squares represent pressure from MgO scales by Speziale et al. (2001) and Jamieson et al. (1982), respectively.

high-pressure and high-temperature experiments. There are significant discrepancies in pressure determination using different pressure standards. The calculated pressures based on different standards could differ as much as 4 GPa at 25 GPa and 2000 K. There is no consistency even within the same pressure standards. For instance, the difference in calculated pressures using Au as the standard can be as large as 2.5 GPa at 25 GPa and 2000 K.

Establishment of a reliable pressure scale is severely hindered by lack of consensus within one pressure standard, regarding the thermal equation of state. The differences are largely due to reliance by some on shock wave data and by others on independently derived thermodynamic parameters. The equations of state for Au by Jamieson et al. (1982) and Anderson et al. (1989) show two end-member cases. Jamieson et al. (1982) relied on the shock wave data alone for the development of the Au scale, whereas Anderson et al. (1989) relied heavily on thermodynamic parameters consistent with high-temperature elasticity measurements at ambient pressure.

With recent advances in synchrotron radiation and high-pressure and high-temperature techniques, static high P-T data have accumulated at an increasingly fast rate. There is an urgent need to develop a practical, reliable pressure scale and to understand the relative differences in pressure by different pressure standards. With COMPRES's support, we have performed high P-T experiments using both multi-anvil apparatus (at Spring-8) and externally-heated diamond-anvil cell (at APS). X-ray diffraction data for multiple internal pressure standards (Au, Pt, MgO) were obtained under simultaneous high P-T conditions up to 28 GPa and 2173 K in the multi-anvil device and up to 56 GPa and 1150 K in the diamond-anvil cell. These data were used to evaluate pressure scales based on the existing equations of state of Au, Pt, and MgO (Fei et al., 2004).

The existing thermal equations of state of pressure standards such as Au, MgO, and Pt, predict a range of pressures at high temperatures for samples under the same pressure and temperature conditions. The maximum differences in the calculated pressures could be as large as 3 GPa at P-T conditions corresponding to the boundary between the transition zone and the lower mantle. The MgO scale of Jamieson et al. (1982), who adopted the thermodynamic parameters given by Carter et al. (1971), predicted the lowest pressure relative to the other pressure scales. This equation of state for MgO does not reproduce more recent static and shock wave data (e.g., Duffy and Ahrens, 1985; Fei, 1999) and should not be used for pressure calculations at high temperatures. Speziale et al. (2001) proposed an equation of state for MgO based on analysis of all available static and shock wave data. The new MgO scale predicts pressures between those of the Au scales of Anderson et al. (1989) and Jamieson et al. (1982), and in general agreement with the results from molecular dynamic simulation of the equation of state of MgO (Matsui et al., 2000). Recently, Shim et al. (2002) pointed out that Anderson et al. (1989) equation of state did not reproduce the shock wave data and Jamieson et al. (1982) used a value for the Grüneisen parameter that is too high. The revised Au scale by Shim et al. (2002) and the MgO scale of Speziale et al. (2001) predict similar pressures at high temperatures. The differences in the calculated pressures by the two pressure scales are about 0.5 GPa at 25 GPa and 2000 K. Using the MgO scale of Speziale et al. (2001) as a practical scale for consistency, we further refine the Au scale

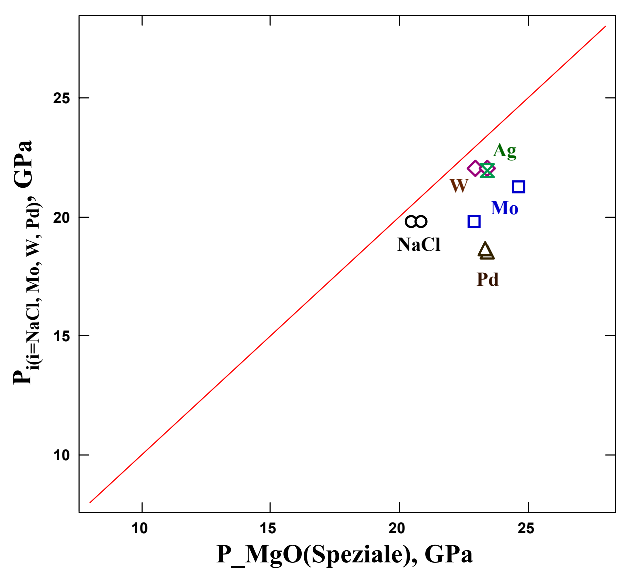

Figure 2. Calculated pressures from the MgO scale of Speziale et al. (2001) compare to the pressures calculated from different internal pressure standards (W, open diamonds; Mo, open squares; Pd, open triangles; Ag, double triangles; and NaCl, open circles) at 1473 K.

of Shim et al. (2002) using our new high P-T data. Our modified Au scale (Fei et al., 2004) gives pressures that are consistent with those calculated from the MgO scale of Speziale et al. (2001). Pressures calculated from the Pt scale of Holmes et al. (1989) and the Au scale of Anderson et al. (1989) give similar pressures at high temperatures. Because pressures calculated from the Au scale of Anderson et al. (1989) are about 1.0 GPa lower than those of Shim et al. (2002) and about 1.5 GPa lower than those from the MgO scale of Speziale et al. (2001) at conditions corresponding to the 660-km discontinuity, the Pt scale underestimates pressures relative to the Au scale of Shim et al. (2002) and the MgO scale of Speziale et al. (2001). We proposed a new thermal equation of state for Pt (Fei et al., 2004) that is consistent with our modified Au scale and the MgO scale of Speziale et al. (2001) as well.

This study provides us with a means to compare high P-T data obtained using different pressure standards such as MgO, Au, and Pt. It is desirable to establish a practical, reliable pressure scale at high temperature while we work toward an absolute pressure scale. The thermal equation of state of MgO is the least controversial one from recent theoretical and experimental studies. We are in favor of using the MgO scale of Speziale et al. (2001) as a reference pressure scale for consistency and inter-laboratory comparison. We further established thermal equations of state for Au and Pt that are consistent with the MgO scale of Speziale et al. (2001).

The ultimate goal for pressure calibration is to establish an absolute pressure scale. Such a goal can be achieved by redundant equation-of-state measurements, i.e. simultaneous density and elasticity determination at high pressure and temperature. These measurements require involvement of experts in both diffraction and elasticity groups. Further inputs from the shock wave community and theoretical group will help us to get close to the goal of establishing an absolute pressure scale.

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President's Message

The first few months of 2004 have been busy ones for the COMPRES community. Following are some highlights of these activities.

The major activity of the Executive Committee in January 2004 was the preparation of the Year #2 Annual Report of COMPRES to the NSF, and the Annual Program Plan and Budget request for Year #3 [May 1, 2004 to April 30, 2005]. In preparation for this submission, the Executive Committee developed a process that involved the COMPRES community and the two elected Standing Committees for Community Facilities and Infrastructure Development Projects. This revised Annual Program Plan and Budget was submitted to the NSF on February 5, 2004. The report, plan and budget for Year #3 [May 1, 2004 to April 30, 2005] was approved by David Lambert of NSF-EAR and the budget increment for Year #3 of $2.2 million authorized. The full Year #2 Annual Report can be viewed on the COMPRES website along with photos which accompanied these reports at the new url: www.compres.us.

In January, the American Geophysical Union announced the 2004 Medallists, Awardees and new Fellows. On behalf of the mineral and rock physics and chemistry communities, COMPRES can point with pride to the members of its extended community who will be honored this year, including:

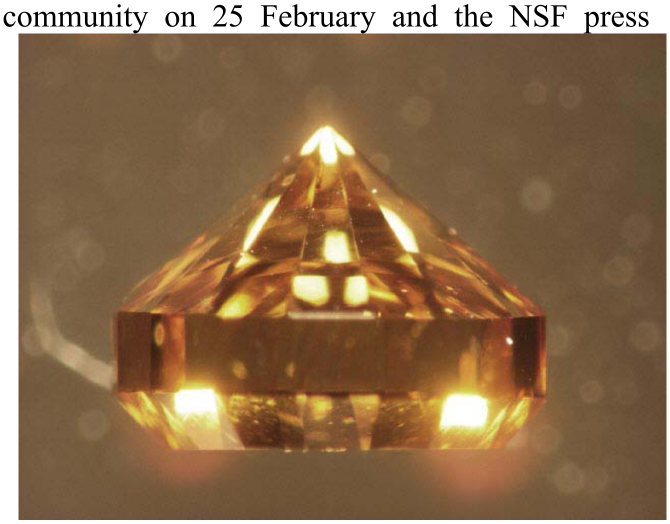
Mervyn Paterson: Walter H. Bucher Medal
Adolphe Nicolas: Harry H. Hess Medal
New AGU Fellows:

- Brian Evans: Massachusetts Institute of Technology
- David Green: Australian National University
- David James: Carnegie Institution of Washington
- Peter Kelemen: Woods Hole Oceanographic Institution
- Michael O'Hara: University of Cardiff
- Allan Rubin: Princeton University
- Ernest Rutter: University of Manchester

Our heartiest congratulations to those to be honored in 2004

On February 21-24, a CSEDI Science Plan Workshop convened by Guy Masters and Cathy Constable was held at the Institute of Geophysics and Planetary Geophysics of the Scripps Institution of Oceanography at the University of California, San Diego in La Jolla. Among the 70+ attendees were 14 from the field of mineral physics. This was an excellent venue for interactions and communications among the scientific disciplines of geodynamics, isotope geochemistry, magnetism, mineral physics, planetary studies and seismology. There were eight outstanding plenary lectures, including two from our colleagues in mineral physics [in the broadest sense], Marc Hirschmann from the University of Minnesota and David Walker from Columbia University. In addition to the Hirschmann and Walker lectures, it was very gratifying to have the experimental and theoretical work in mineral physics highlighted in the other lectures by David Stevenson, Peter Olson, Louise Kellogg, Rob van der Hilst, Peter van Keken and Ed Garnero. Bob Liebermann gave a brief presentation on the new COMPRES consortium, as one example of organized research activities in Earth Sciences sponsored by the NSF.

The research team at the Carnegie Institution of Washington and the Los Alamos National Laboratory reported a major breakthrough in growing diamonds from chemical vapor deposition. (see Photo below) They found that the high-P-T annlealed crystals are the hardest known to date C-s. Yan, H-k. Mao, W. Li, J. Qian, Y. Zhao and R. J. Hemley in phys. stat. solidi (a) 201, R25 (2004). [see the separate email sent to the COMPRES community on 25 February and the NSF press



release attached]. This achievement is a product of one of the Grand Challenge collaborative research proposals which were submitted and funded by the NSF Division of Earth Sciences in 2002. While these collaborative projects are officially distinct from the COMPRES Core grant, they are closely linked on an intellectual level in that they provide some of the basic scientific rationale for developing and maintaining the experimental facilites overseen and operated under the auspices of COMPRES.

A COMPRES/GSECARS Workshop on "Future Directions for the Laser-Heated Diamond Cell at the Advanced Photon Source " was held on March 20, 2004 at the APS of ANL, convened by Thomas Duffy (Princeton), Guoyin Shen (Chicago) and Dion Heinz (Chicago) who are leading the COMPRES Infrastructure Development Project on "Laser-Heated Diamond Anvil Cell." The Workshop was attended by 40 people. Copies of the presentations at the Workshop may be found on the COMPRES website.

The Institut de Physique du Globe de Paris hosted a one-day symposium on “Physique des minéraux” in honor of Jean-Paul Poirier, who retired in May 2003. Convened by François Guyot and Philippe Gillet, the program included presentations by former French students and colleagues of Poirier [A. Nicolas, G. Fiquet, J. Ingrin, S. Labrosse, D. Andrault, C. Sotin, P. Gillet, and C. Allegre] as well as a few l’étranger [T. Shankland, D. Price, F. Langenhorst, and R. Liebermann]. See right for details of the program.

A COMPRES Workshop on “Focused Ion Beam Milling" was held on March 27-28 at the Mission Inn in Riverside, California, convened by Harry Green of the University of California at Riverside. The Workshop was attended by over 50 participants, who were able to see a demonstration instrument set up by one of the manufacturers. A full report of the Workshop will be posted soon on the COMPRES website.

In April 2003, the bid for Approved Program (AP) status from High Pressure COMPRES team at the Advanced Light Source of the Lawrence Berkeley National Laboratory [R. Jeanloz, S. Clark, M. Kunz] was approved by the ALS Advisory Committee. Simon Clark was recently informed that the ALS will allocate 20 percent of the beamtime on beamlines 1.4 and 11.3.1 to their team for the period July 2004 until June 2007.

The Advisory Committee for COMPRES [Bruce Buffett, Chi-chang Kao, Guy Masters, Richard O’Connell, and Paul Silver] will meet at Granlibakken Resort on Saturday, June 19 with the Executive Committee.

Best regards,
Bob Liebermann

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Welcome New Members of COMPRES

In March 2004, COMPRES welcomed the following institutions to membership in COMPRES:

University of New Mexico
Elector: Carl Agee
Alternate: David Draper

Tohoku University in Sendai, Japan
Representative: Eiji Ohtani

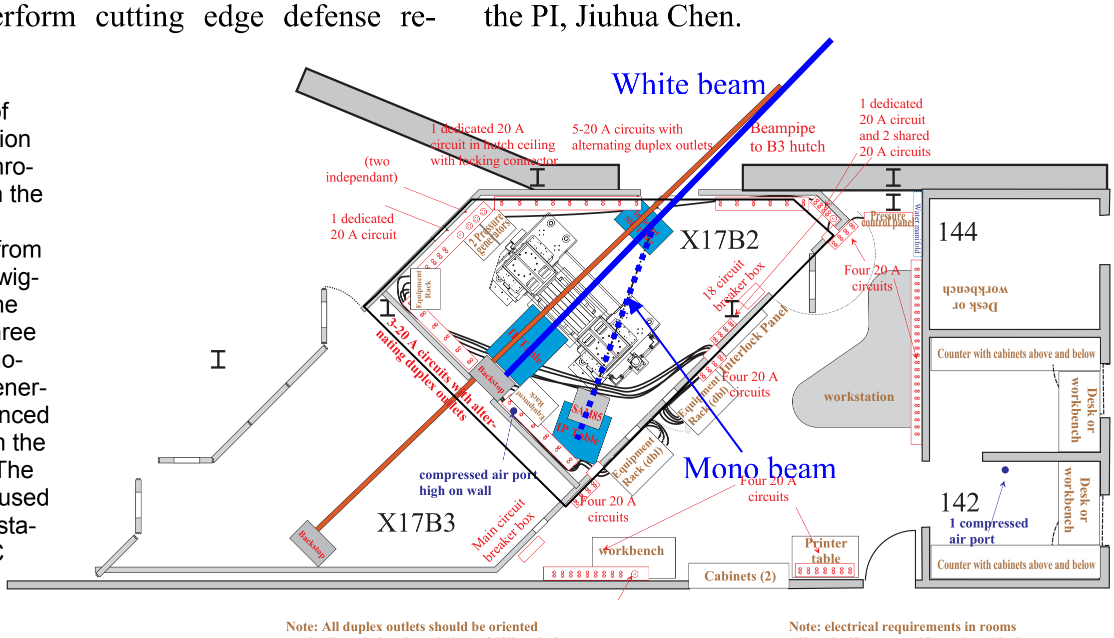
Ruhr-Universität Bochum, Bochum, Germany
Representative: Sumit Chakraborty

Universität Bayreuth, Bayreuth, Germany:
Representative: David Rubie

This brings the total institutional membership to 39 U. S. institutions and a 11 foreign affiliates. A complete list can be found on the COMPRES website, where you will also find US and world maps showing the locations of these member institutions.

DoD Investment to COMPRES Facility

Department of Defense recently awarded an instrumentation project proposed by Jiuhua Chen and Donald Weidner of Stony Brook to complement COMPRES high pressure facility for melt property studies at the X17B2 beamline of the National Synchrotron Light Source at the Brookhaven National Laboratory. The project is awarded under the Defense University Research Instrumentation Program (DURIP). This program supports the purchase of state-of-the-art equipment that augments current university capabilities or develops new university capabilities to perform cutting edge defense research. The project is funded at a level of $200,000 for installing an on-line imaging plate detector to establish a monochromatic x-ray side-station. This new experimental station is designed to run simultaneously with the existing white x-ray station, therefore increases the available beam time for high pressure study and enables new experimental capabilities. “NSF research grants through EAR program have played a critical role in supporting the research that demonstrates the importance of such a monochromatic x-ray station in the proposal”, said the PI, Jiuhua Chen.



Conceptual design of simultaneous operation of white and monochromatic x-ray station in the X17B2 hutch at the NSLS. White beam from the superconductor wiggler is delivered to the hutch splitting into three subbeams. The monochromatic x-ray is generated by a single bounced monochromator from the center white beam. The two side beams are used by the X17B2 white station and X17B3 DAC station.

Recent PhDs

Kanani Kealaokehaulani Meulang Lee,

Ph. D. 2003,

University of California, Berkeley

Dissertation**: Exploring Planetary Interiors: Experiments at Extreme Conditions**

In-situ high-pressure and high-temperature experiments are invaluable to understanding the interiors of planets primarily giving us insight into the relationship of pressure and temperature on the chemical and physical characteristics of planetary materials as well as testing current theories of planetary accretion, differentiation and evolution throughout a planet's lifetime.

X-ray diffraction was used to measure the volume response to pressure and temperature of a natural peridotite at lower-mantle pressures. A lower mantle composed of an upper-mantle rock composition is 1-4% less dense than seismic observations for temperatures between 2000-3000 K, suggesting distinct mantle layers not only based on structural phase changes but also chemical differences.

X-ray diffraction was also used to track the alloying behavior between two very different elements, alkali-metal potassium (K) and transition-metal iron (Fe) to test the theory of an alkali-to-transition metal electronic transition at high pressure as well as the theory of sequestering potassium into the Earth's iron-rich core thereby providing a long-lived radioactive isotope ^{40}K to power the Earth's magnetic field and mantle dynamics. At pressures above ~26 GPa and above the melting temperature of iron, K and Fe form an alloy in which one percent of the Fe atoms are substituted for K in the hexagonal close-pack structure of ε-Fe thereby validating the former theory and making the latter possible.

Dynamic and static experimental methods were combined to explore the behavior of water at pressures above ~50 GPa and up to ~10,000 K. Water is found to exhibit complicated physical behavior—not surprising since at relatively low pressures and temperatures water has more than a dozen structures—with changing optical properties indicative of ionization and metallization with increased pressures and temperatures.

Statement

My experiences as a graduate student working with Raymond Jeanloz (University of California, Berkeley) and Gilbert Collins (Lawrence Livermore National Laboratory) were excellent. I was given the flexibility to work on a number of planetary materials (peridotite, iron-potassium alloying, and water) at high pressures and temperatures thus allowing me to research my varied interests in my thesis entitled, "Exploring Planetary Interiors: Experiments at Extreme Conditions." I am currently an O. K. Earl Postdoctoral Fellow at the California Institute of Technology working with Paul Asimow and Tom Ahrens on lower-mantle assemblages. I am also continuing collaborations with Gerd Steinle-Neumann at Bayerisches Geoinstitut at the University of Bayreuth using ab-initio calculations to further understand Fe-alloying processes under high compression.

COMPRES Upcoming Events

2004 Annual Meeting of COMPRES

The 2004 COMPRES Annual Meeting will be held at the Granlibakken Conference Center and Resort in Lake Tahoe, California from June 20-22, 2004. [Arrivals on June 19/Departures on June 22] Please mark your calendars for this important COMPRES event. You can find more information on this meeting at on the COMPRES website, including the tentative program and agenda. Additional details of the Granlibakken resort may be found at: http://www.granlibakken.com/.

Rheology Grand Challenge Workshop

Organized by Shun-ichiro Karato, a Rheology Grand Challenge Workshop will be held at Yale University, New Haven, on May 2. Contact shun-ichiro.karato@yale.edu for more details.

Elasticity Grand Challenge Workshop

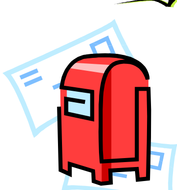
Organized by Jay Bass, an Elasticity Grand Challenge Workshop will be held at the University of Illinois at Urbana-Champaign on May 8. Contact Jaybass@uiuc.edu for more details.

Opportunities

Post-doctoral Research Associate

The Department of Geology, University of Illinois at Urbana-Champaign, seeks a post-doctoral research associate to participate in synchrotron radiation studies on materials under high pressure and high temperature conditions. The position will be located at sector 3 of the Advanced Photon Source, which offers unique scientific opportunities related to investigations of iron-bearing minerals and alloys under extreme conditions using nuclear resonant scattering. Experience with synchrotron radiation techniques is required. Experience with diamond anvil high-pressure cells and laser-heating techniques is desireable, as is a basic knowledge of inelastic neutron or x-ray scattering, or nuclear resonant scattering. The position will involve the design and testing of high-pressure and high-temperature instrumentation, interacting with beamline users in the planning and execution of their experiments, the analysis and publication of results, and organizing community information/outreach activities. The position presents an opportunity to contribute to the prominent and unique nuclear resonant scattering program of the Advanced Photon Source by developing techniques that are of particular interest for the high-pressure and Earth-science community. The position is available as of July 1, 2004.

For additional information contact either Dr. Wolfgang Sturhahn, (630) 252-0163, sturhahn@aps.anl.gov or Dr. Jay Bass, (217) 333-1018, jaybass@uiuc.edu. Applicants should send a CV, a statement of experience and research interests, list of publications, and arrange to have three letters of recommendation sent to Dr Jay Bass, Department of Geology, University of Illinois, 1301 W Green St., Urbana, IL 61801 USA. The University of Illinois is an Affirmative Action/Equal Opportunity employer. Women, minorities, and other designated classes are encouraged to apply.



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