Russell Hemley and Ho-kwang Mao

Russell J. Hemley is Senior Staff Scientist at the Geophysical Laboratory of the Carnegie Institution, Washington DC and Director of the Carnegie/DOE Alliance Center (CDAC)

Ho-kwang Mao is Senior Staff Scientist at the Geophysical Laboratory of the Carnegie Institution, Washington DC

2005 Balzan Prize for Mineral Physics

For the impressive impact of their joint work leading to fundamental breakthroughs, theoretical and experimental, in the field of minerals submitted to extreme physical conditions. They have operated as a highly effective team, characterized by twenty years of research contributions at the highest level. They have developed techniques which allow them to study the behaviour of a wide range of materials, such as hydrogen, the most abundant "mineral" in the universe. Their results have deep implications for our understanding of nature.

Institution Administering Research Funds:

Carnegie Institution of Washington, Geophysical Laboratory

Adviser for the Balzan General Prize Committee: Enric Banda

New Directions in Mineral Physics: Multidisciplinary High Pressure Science

With the second half of their Balzan Prize, Russell Hemley and Ho-kwang Mao implemented a project focused on bringing bright young people from diverse backgrounds into the multidisciplinary field of High Pressure Science. Recent advances in mineral physics are unleashing the power of high pressure research to tackle a broad range of great challenges that span numerous scientific disciplines. Breakthroughs are expected in applications of high pressure research to mineralogy, geophysics, geochemistry and bioscience, as well as specific areas such as hydrogen storage, superhard materials and superconductivity. We are thus coming close to solving mysteries like the Earth's inner core and the roots of plate tectonics. The project was focused on training and its goal was the exploration of the new high-pressure

dimension in multidisciplinary physical sciences. The fellowships encouraged the development, design, and fabrication of new instrumentation that exploited the CVD diamond technology developed by Professors Hemley and Mao. Publications and dissemination of results have also being financed.

- Dr. Pierre Beck was a Balzan Prize supported post-doctoral associate from 2006-2007. He was trained in high-pressure meteorite impact phenomena at the Ecole Normale Superieure in Lyon, France. Prior to joining Professors Hemley and Mao, he published a series of papers on meteorite studies including an important article in "Nature" in 2005. As part of his Balzan-supported project, he developed time-resolved (i.e. dynamic) high pressure-temperature phenomena with diamond anvil cells. His work has led to the first high pressure-temperature Raman studies of olivine and to a novel method for measuring the thermal conductivity of materials at high pressures and temperatures, with two papers and a series of abstracts in press. This is part of Professors Hemley and Mao's Balzan-supported project to develop combined static and dynamic (i.e. shock-wave) compression science.
- Dr. Lin Wang was a Balzan Prize supported post-doctoral associate who received his Ph.D. degree from Jilin University, China. He developed a new method for the synthesis of controlled shape C60 fullerene nanorods. Further high-pressure/ temperature treatments lead to polymerization and transitions to tetragonal, orthorhombic, or rhombohedral phases. These nanorods exhibit very rich nano effects in their optical, structural, phase transition, and compressional properties but lack an in situ probe to characterize the structure directly. Dr. Wang developed a new technique to integrate the high-pressure diamond anvil cell with the high brilliance x-ray beam focused down to 50-200 nm size at the Advanced Photon Source. This will open a new field of single-crystal x-ray nanocrystallography that will explore the correlation between crystal structure, dimensionality, and size of nanomaterials under high pressures. With Balzan Award support, Dr. Lin Wang has been working at the High Pressure Synergetic Consortium (HPSynC) at the Advanced Photon Source (APS), Argonne National Laboratory (ANL) in 2008. He is pioneering the x-ray nanocrystallographic studies that explore the correlation between crystal structure, dimensionality, and size of nanomaterials under high pressures.
- Mr. Charles Qiaoshi Zeng received Balzan Prize support from 1st September to 31st
 December 2008. Mr. Zeng was a pre-doctoral fellow from Zhejiang University,

China, who had done a superb job both at the Geophysical Laboratory and APS. Mr. Zeng has conducted numerous x-ray diffraction experiments at the APS synchrotron facility. Most recently, he has discovered a new type of alloy and a new phenomenon in metallic glass that have far-reaching impact in fundamental physics as well as materials applications. This discovery, published in PNAS as "Novel Substitutional Alloy of Ce and Al" was selected "In This Issue" section highlights particularly interesting articles published in the print issue of PNAS, 24th February 2009.

Several high school students who also received Balzan Award support are Andrew Kung, Daniel Cohen, Alexander Levedahl, Claire Barkett, Maura James, Manchali Madurri, and Jaqueline Rivera.

- Mr. Andrew Kung was a high school student who received Balzan Prize support to develop a high-pressure project studying the pressure, temperature, and temporal effects on a newly discovered O₂-H₂ alloy. This alloy was synthesized by compressing water into high-pressure phase ice VII and irradiated by x-rays, splitting the H₂O molecules into O₂ and H₂. At ordinary pressure, O₂ reacts explosively with H₂ to form H₂O, but they coexist stably at high pressures. Mr. Kung used Raman spectroscopy as an in situ diagnostic probe to find the amounts of O₂ and H₂ in the alloy and their changes with pressure, temperature, and time. The study provides important information about this novel material and its possible energy and environmental applications.
- Mr. Daniel Cohen was a high school student who received Balzan Award support to study novel electronic phenomena in diamond. Professors Hemley and Mao have extended their previous methods for growing large single crystal diamond by chemical vapor deposition (CVD) to include very high levels of doping with nitrogen. The goal of Mr. Cohen's project is to produce a new material with metallic electrical conductivity, and possibly superconductivity. The project involved careful measurement of electrical resistivity as a function of temperature from 4-500 K of well characterized nitrogendoped CVD diamond that Professors Hemley and Mao produce in their laboratory.
- Mr. Alexander Levedahl was a high school student who received Balzan Prize support to investigate the high pressure-temperature behavior of hydrogen-containing ice materials known as hydrogen clathrates. These newly discovered materials are important for a broad range of problems, including understanding planetary evolution and climate change, as well as the development of new hydrogen storage materials.

147

The experiments use laser spectroscopy techniques to determine the melting curve and new possible high pressure-temperature solid phases containing H_2 and H_2O .

- Ms. Claire Barkett was a high school student at Good Counsel High School in Olney, MD and was at Carnegie during the 2008-2009 school year. Ms. Barkett received Balzan Prize support as she followed up on the earlier work of Jaqueline Rivera by synthesizing several solid solutions in the Fe₂O₃-Al₂O₃ system very close to the 1:1 FeAlO₃ composition. Because FeAlO₃ has a completely different structure to the rest of the Fe₂O₃-Al₂O₃ join, which have a rhombohedral corundum structure, which is isostructural to the end members, it is of interest to know the precise range of compositions where the FeAlO₃ structure is stable. The careful chemical synthesis methods developed and carried out in this work were therefore crucial. Diffraction measurements on these materials allowed a refinement of work carried out in the 1950s, and a better understanding the role of magnetic interactions between ferric ions in stabilizing the FeAlO₃ structure.
- Ms. Maura James received Balzan Prize support in the summer of 2008. Ms. James was a high school student from the Convent of the Sacred Heart in Greenwich, CT. She investigated high pressure clathrate formation in the H₂O-NH₂- H₂ ternary system with Stephen Gramsch and Maddury Somayazulu. This was an exploratory project in which Ms. James worked out special techniques for sample loading and mapping the composition of the mixture inside the diamond anvil cell. Using Raman spectroscopy, she found that with increasing pressure, the ammonium hydroxide-H₂ mixture separates into two phases, a water-rich phase and an ammonia-rich phase that appears be composed of a clathrate containing the hydrogen molecules.
- Ms. Manchali Madurri was a high school student at Thomas Jefferson High School in Alexandria, VA. Ms. Madurri received Balzan Prize support in the summer of 2008 for her study of H₂-crown ether complexes at high pressure. Using Raman spectroscopy to track the vibrational properties of both the crown ether host and the complexed hydrogen molecules, she found that crown ether-hydrogen complexation is promoted by applied pressure, and that the optimal crown ether ring size for effective complexation of hydrogen is approximately 1.7-2.2 Å. This complexation appears to be enhanced upon decompression from pressures of approximately 5GPa, a result that has important implications for the use of such materials in hydrogen storage applications. As a result of her work, Ms. Madurri was named a

semifinalist in both the Intel and Siemens national science fair competitions.

- Ms. Jaqueline Rivera was a high school student from the Cesar Chavez High School in Washington, DC and received Balzan Prize support during the summer of 2008. Ms. Rivera developed new room-temperature, solution-based synthesis methods for solid solutions in the Fe₂O₃-Al₂O₃ solid solution system. These methods ensure that the resulting material is as homogeneous as possible, but allow precise control of composition. This particular series of compounds can serve as a model system for understanding the effect of aluminum on the concentration of ferric iron, ferrous iron and oxygen vacancies in deep mantle minerals, particularly silicate perovskite and post-perovskite. The concentration and role of ferric iron in the deep mantle has important consequences for many high-pressure mineral properties. Ms. Rivera subsequently went on to study biochemistry at the Catholic University of America.

Presentations:

- Beck, P., A. F. Goncharov, V. Struzhkin, B. Militzer and R. J. Hemley, *Measurements of thermal diffusivites under planetary interiors pressure temperature conditions*, 2007 Stewardship Science Academic Alliances Program Symposium (Washington, DC, 5th-7th February 2007).
- Somayazulu, M., A. Levedahl, S. Scott, S. Gramsch, H. K. Mao and R. J. Hemley, High pressure-temperature Raman spectroscopy of H₂-H₂O clathrate. Geophysical Laboratory, Carnegie Institution of Washington, March Meeting of the American Physical Society, Denver, CO, March 2007. Link: http://meetings.aps.org/link/BAPS.2007.MAR.D23.6
- Liang, Q., C. S. Yan, Y. Meng, J. Lai, S. Krasnicki, T. Yu, H. Shu, H. K. Mao, and R. J. Hemley, *Ultratough single crystal diamonds by MPCVD*, Intertech 2008 (Orlando, FL, 5th-7th May 2008).
- Liang, Q., C. S. Yan, Y. F. Meng, J. Lai, S. Krasnicki, T. Yu, H. Shu, H. K. Mao, and R. J. Hemley, *Recent progress in fabrication of high quality single crystal diamond at high growth rates*, Lithosphere petrology and origin of diamond International Symposium (Novosibirsk, Russia, 5th-7th June 2008).
- Meng, Y. F., C. S. Yan, J. Lai, S. Krasnicki, H. Y. Shu, T. Yu, Q. Liang, H. K. Mao and R. J. Hemley, *High-temperature/low-pressure annealing of SC-CVD diamond*, 2nd International Conference on New Diamond and Nano Carbons (NDNC2008) (Taiwan, 26th-29th May 2008).

Researchers:

Pierre Beck post-doctoral associate Lin Wang post-doctoral associate

Charles Qiaoshi Zeng pre-doctoral fellow

Claire Barkett high school student
Daniel Cohen high school student
Maura James high school student
Andrew Kung high school student
Alexander Levedahl high school student
Manchali Madurri high school student
Jaqueline Rivera high school student

Publications (in chronological order):

- Beck, P., A. F. Goncharov, and R. J. Hemley, *High-pressure high temperature Raman spectroscopy of San Carlos olivine*, Eos Trans. AGU Fall Meet., Suppl., 87, 2006.
- Banighan, E. J., R. Caracas, P. Beck, and R. J. Hemley, *Theoretical and experimental Raman study of spinel*, Eos Trans. AGU Fall Meet., Suppl., 87, 2006.
- Somayazulu, M., Levedahl, A., Goncharov, A., Mao, H.-K. and Hemley, R.J. 2007.
 High-pressure-temperature Raman spectroscopy of H₂-H₂O clathrate [Abstract].
 Bulletin of the American Physical Society, 52(1).
- Beck, P., A. F. Goncharov, V. V. Struzhkin, B. Militzer, H.-K. Mao, and R. J. Hemley, *Measurement of thermal diffusivity at high pressure using a transient heating technique*, Appl. Phys. Lett., 91, 181914, 2007.
- Meng, Y. F., C. S. Yan, J. Lai, S. Krasnicki, H. Shu, Q. Liang, H.-K. Mao, and R. J. Hemley, Enhanced optical properties of chemical vapor deposited single crystal diamond by low-pressure/high-temperature annealing, Proc. Nat. Acad. Sci., 105, 17620-17625, 2008.
- Goncharov, A. F., B. Haugen, V. V. Struzhkin, P. Beck, and S. D. Jacobsen, *Radiative conductivity and oxidation state of iron in the Earth's lower mantle*, Nature, 456, 231-234, 2008.
- Liu, H., L. Wang, X. Xiao, F. De Carlo, J. Feng, H.-K. Mao, and R. J. Hemley, *Anomalous pressure-induced behavior of amorphous selenium from synchrotron x-ray diffraction and microtomography*, Proc. Nat. Acad. Sci., 105, 13229-13234, 2008.

- Goncharov, A. F., P. Beck, V. V. Struzhkin, R. J. Hemley, and J. C. Crowhurst, *Laser heating diamond anvil cell studies of simple molecular systems at high pressures and temperatures*, J. Phys. Chem. Solids, 69, 2217-2222, 2008.
- Goncharov, A. F., S. D. Jacobsen, V. V. Struzhkin, and P. Beck, Optical properties of minerals in the deep-earth, in McGraw Hill 2008 Yearbook of Science & Technology 242-245, McGraw Hill, New York, 2008.
- Jia, L., J. R. Sun, F. W. Wang, T. Y. Zhao, H. W. Zhang, B. G. Shen, D. X. Li, S. Nimori, Y. Ren, and Q. S. Zeng, *Volume dependence of the magnetic coupling in LaFe*_{13-x}Si_x based compounds, Appl. Phys. Lett., 92, 101904, 2008.
- Zeng, Q., Z. He, X. San, Y. Ma, F. Tian, T. Cui, B. Liu, G. Zou, and H.-K. Mao, *A new phase of solid iodine with different molecular covalent bonds*, Proc. Nat. Acad. Sci., 105, 4999-5001, 2008.
- Goncharov, A. F., P. Beck, V. V. Struzhkin, B. D. Haugen, and S. D. Jacobsen, *Thermal conductivity of lower mantle minerals*, Phys. Earth Planet. Inter., 174, 24-32, 2009.
- Liang, Q., C. Y. Chin, J. Lai, C. S. Yan, Y. F. Meng, H.-K. Mao, and R. J. Hemley, Enhanced growth of high quality single crystal diamond by MPCVD at high gas pressures, Appl. Phys. Lett., 94, 024103, 2009.
- Sun, L., W. Yi, L. Wang, J. Shu, S. Sinogeikin, Y. Meng, G. Shen, L. Bai, Y. Li, H.- K. Mao, and W. L. Mao, *X-ray diffraction studies and equation of state of methane at 200 GPa*, Chem. Phys. Lett., 473, 72-74, 2009.
- Wang, L., Y. Pan, Y. Ding, W. Yang, W. L. Mao, S. V. Sinogeikin, Y. Meng, G. Shen, and H.-K. Mao, *High-pressure induced phase transitions of Y*₂*O*₃ and Y₂*O*₃:*Eu*³⁺, Appl. Phys. Lett., 94, 061921, 2009.
- Wang, L., Y. Ding, W. Yang, W. L. Mao, W. Liu, Z. Cai, J. Shu, G. Shen, and H.-K. Mao, *Application of nano/submicron-focused x-ray probe for ultrahigh-pressure studies*, High Pressure Synchrotron Science Workshop (Argonne, IL, 6th-8th May 2009).
- Zeng, Q. S., Y. Ding, W. L. Mao, W. Luo, A. Blomqvist, R. Ahuja, W. Yang, J. Shu, S. V. Sinogeikin, Y. Meng, D. L. Brewe, J. Z. Jiang, and H.-K. Mao, *Substitutional alloy of Ce and Al*, Proc. Nat. Acad. Sci., 106, 2515-2518, 2009.
- Liang, Q., C. S. Yan, Y. Meng, J. Lai, S. Krasnicki, H.-K. Mao, and R. J. Hemley, *Recent advances in high-growth rate single-crystal CVD diamond*, "Diamond and Related Materials", Volume 18, 2009, 698-703.
- Liang, Q., C. S. Yan, Y. Meng, J. Lai, S. Krasnicki, T. Yu, H. Shu, H.-K. Mao and R.J. Hemley, *Ultratough single crystal diamonds by MPCVD*, Proceedings of Intertech 2008.

- Liang, Q., C. S. Yan, Y. F. Meng, J. Lai, S. Krasnicki, H.-K. Mao, and R. J. Hemley, Enhancing the mechanical properties of CVD single-crystal diamond, "Journal of Physics: Condensed Matter", Issue 36, 9th September 2009.
- Beck, P., A. F. Goncharov, J. A. Montoya, V. V. Struzhkin, B. Militzer, R. J. Hemley, and H.-K. Mao, *Response to "Comment on 'Measurements of the thermal diffusivities at high-pressure using a transient heating technique'"*, "Applied Physical Letters", Volume 95, Issue 9, August 2009.
- Zha, C. S., S. Krasnicki, Y. F. Meng, C. S. Yan, J. Lai, Q. Liang, H.-K. Mao, and R. J. Hemley, Composite chemical vapor deposition diamond anvils for highpressure/high-temperature experiments, "High Pressure Research", Volume 29, Issue 2, June 2009.
- Liang, Q., C. S. Yan, Y. F. Meng, J. Lai, T. Yu, H. Shu, S. Krasnicki, H.-K. Mao, and R. J. Hemley, *Evidence for ultratough single crystal CVD diamond*, Phys. Stat. Sol. (forthcoming).
- Liang, Q., C. S. Yan, Y. Meng, J. Lai, S. Krasnicki, T. Yu, H. Shu, H.-K. Mao and R. J. Hemley, *Ultratough boron-doped CVD single-crystal diamond*, Adv. Mat. (submitted).
- Beck, P., A. F. Goncharov, V. V. Struzhkin, B. Militzer, R. J. Hemley, and H.-K. Mao, *Measurements of thermal diffusivity under pressure in the diamond-anvil cell*, Appl. Phys. Lett. (to be submitted).
- Somayazulu, M., Levedahl, A., Scott, S., Gramsch, S., H.-K. Mao and R. J. Hemley, *High pressure-High temperature Raman spectroscopy of C2 clathrate of H*₂-H₂O (to be communicated).
- Beck, P., A. F. Goncharov, H.-K. Mao, and R. J. Hemley, *High pressure and temperature Raman spectroscopy of olivine*, Geophys. Res. Lett. (in preparation).