Russell Hemley and Ho-kwang Mao

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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 multi-

disciplinary 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 been 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 École 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 PhD 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 nanoeffects 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 1 September to 31 December 2008. Mr. Zeng was a pre-doctoral fellow from Zhejiang University, China, and 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 was published in the 24 February 2009 issue of PNAS as "Substitutional Alloy of Ce and Al".

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

- Mr. Andrew Kung received Balzan Prize support to develop a high-pressure project studying the pressure, temperature and temporal effects on a newly discovered O_2-H_2 alloy. This alloy was synthesized by compressing water into high-pressure phase ice VII and irradiated by x-rays, splitting the H_2O molecules into O_2 and H_2. At ordinary pressure, O_2 reacts explosively with H_2 to form H_2O, but they coexist stably at high pressures. Mr. Kung used Ramanspectroscopy as an in situ diagnostic probe to find the amounts of O_2 and H_2 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 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 nitrogen doped CVD diamond that Professors Hemley and Mao produce in their laboratory.

- Mr. Alexander Levedahl 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. 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 attended high school at Good Counsel High School in Olney, MD and was at Carnegie during the 2008-2009 school year. She received Balzan Prize support as she followed up on the earlier work of Jaqueline Rivera by synthesizing several solid solutions in the Fe_2O_3-Al_2O_3 system very close to the 1:1 $FeAlO_3$ composition. Because $FeAlO_3$ has a completely different structure to the rest of the Fe_2O_3-Al_2O_3 join, which have a rhombohedral corundum structure that is isostructural to the end members, it is of interest to know the precise range of compositions where the $FeAlO_3$ 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 of the role of magnetic interactions between ferric ions in stabilizing the $FeAlO_3$ structure.

- Ms. Maura James received Balzan Prize support in the summer of 2008 when she was a high school student from the Convent of the Sacred Heart in Greenwich, CT. She investigated high pressure clathrate formation in the H_2O-NH_2-H_2 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-H_2 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 when she received Balzan Prize support in the summer of 2008 for her study of H_2-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 went to high school at 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 Fe_2O_3-Al_2O_3 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, Goncharov AF, Struzhkin V, Militzer B, Hemley RJ. *Measurements of thermal diffusivites under planetary interiors pressure temperature conditions*. 2007 Stewardship Science Academic Alliances Program Symposium (Washington, DC, 5-7 February 2007).
- Somayazulu M, Levedahl A, Scott S, Gramsch S, Mao HK, Hemley RJ. *High pressure-temperature Raman spectroscopy of H_2-H_2O 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, Yan CS, Meng Y, Lai J, Krasnicki S, Yu T, Shu H, Mao HK, Hemley RJ. *Ultratough single crystal diamonds by MPCVD*. Intertech 2008 (Orlando, FL, 5-7 May 2008).
- Liang Q, Yan CS, Meng YF, Lai J, Krasnicki S, Yu T, Shu H, Mao HK, Hemley RJ. *Recent progress in fabrication of high quality single crystal diamond at high growth rates*. Lithosphere petrology and origin of diamond International Symposium (Novosibirsk, Russia, 5-7 June 2008).
- Meng YF, Yan CS, Lai J, Krasnicki S, Shu HY, Yu T, Liang Q, Mao HK, Hemley RJ. *High-temperature/low-pressure annealing of SC-CVD diamond*. 2 International Conference on New Diamond and Nano Carbons (NDNC2008). (Taiwan, 26-29 May 2008).

Researchers:

Pierre Beck
Lin Wang
Charles Qiaoshi Zeng

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

Publications:

Beck P, Goncharov AF, Hemley RJ-2006. High-pressure high temperature Raman spectroscopy of San Carlos olivine. Eos Trans. AGU Fall Meet., Suppl., 87.

Banighan EJ, Caracas R, Beck P, Hemley RJ. 2006. Theoretical and experimental Raman study of spinel. Eos Trans. AGU Fall Meet., Suppl., 87.

Somayazulu M, Levedahl A, Goncharov A, Mao HK, Hemley RJ. 2007. High-pressure-temperature Raman spectroscopy of H_2-H_2O clathrate [Abstract]. Bulletin of the American Physical Society, 52(1).

Beck P, Goncharov AF, Struzhkin VV, Militzer B, Mao HK, Hemley RJ. 2007. Measurement of thermal diffusivity at high pressure using a transient heating technique. Appl. Phys. Lett., 91: 181914.

Meng YF, Yan CS, Lai J, Krasnicki S, Shu H, Liang Q, Mao HK, Hemley RJ. 2008. Enhanced optical properties of chemical vapor deposited single crystal diamond by low-pressure/high-temperature annealing. Proc. Nat. Acad. Sci., 105: 17620-17625.

Goncharov AF, Haugen B, Struzhkin VV, Beck P, Jacobsen SD. 2008. Radiative conductivity and oxidation state of iron in the Earth's lower mantle. Nature 456: 231-234.

Liu H, Wang L, Xiao X, De Carlo F, Feng J, Mao HK, Hemley RJ. 2008. Anomalous pressure-induced behavior of amorphous selenium from synchrotronx-ray diffraction and microtomography. Proc. Nat. Acad. Sci., 105: 13229-13234.

Goncharov AF, Beck P, Struzhkin VV, Hemley RJ, Crowhurst JC. 2008. Laser heating diamond anvil cell studies of simple molecular systems at high pressures and temperatures. J. Phys. Chem. Solids, 69: 2217-2222.

Goncharov AF, Jacobsen SD, Struzhkin VV, Beck P. 2008. Optical properties of minerals in the deep-earth. McGraw Hill 2008 Yearbook of Science & Technology, 242-245. New York: McGraw Hill.

Jia L, Sun JR, Wang FW, Zhao TY, Zhang HW, Shen BG, Li DX, Nimori S, Ren Y, Zeng QS. 2008. Volume dependence of the magnetic coupling in $LaFe_{13-x}Si_x$ based compounds. Appl. Phys. Lett., 92: 101904, 2008.

Zeng Q, He Z, San X, Ma Y, Tian F, Cui T, Liu B, Zou G, Mao HK. 2008. A new phase of solid iodine with different molecular covalent bonds. Proc. Nat. Acad. Sci., 105: 4999-5001.

Liang Q, Yan CS, Meng Y, Lai J, Krasnicki S, Yu T, Shu H, Mao HK, Hemley RJ. 2008. Ultratough single crystal diamonds by MPCVD. Proceedings of Intertech 2008.

Goncharov AF, Beck P, Struzhkin VV, Haugen BD, Jacobsen SD. 2009. Thermal conductivity of lower mantle minerals. Phys. Earth Planet. Inter. 174: 2432.

Liang Q, Chin CY, Lai J, Yan CS, Meng YF, Mao HK, Hemley RJ. 2009. Enhanced growth of high quality single crystal diamond by MPCVD at high gas pressures. Appl. Phys. Lett. 94: 024103.

Sun L, Yi W, Wang L, Shu J, Sinogeikin S, Meng Y, Shen G, Bai L, Li Y, Mao HK, Mao WL. 2009. X-ray diffraction studies and equation of state of methane at 200 GPa. Chem. Phys. Lett. 473: 72-74.

Wang L, Pan Y, Ding Y, Yang W, Mao WL, Sinogeikin SV, Meng Y, Shen G, Mao HK. 2009. High-pressure induced phase transitions of Y_2O_3 and Y_2O_3:Eu^{3+}. Appl. Phys. Lett., 94: 061921.

Wang L, Ding Y, Yang W, Mao WL, Liu W, Cai Z, Shu J, Shen G, Mao HK. 2009. Application of nano/submicron-focused x-ray probe for ultrahigh-pressure studies. High Pressure Synchrotron Science Workshop (Argonne, IL, 6-8 May 2009).

Zeng QS, Ding Y, Mao WL, Luo W, Blomqvist A, Ahuja R, Yang W, Shu J, Sinogeikin SV, Meng Y, Brewe DL, Jiang JZ, Mao HK. 2009. Substitutional alloy of Ce and Al. Proc. Nat. Acad. Sci. 106: 2515-2518.

Liang Q, Yan CS, Meng Y, Lai J, Krasnicki S, Mao HK, Hemley RJ. 2009. Recent advances in high-growth rate single-crystal CVD diamond. Diamond and Related Materials. Volume 18: 698-703.

Liang QC, Yan S, Meng YF, Lai J, Krasnicki S, Mao HK, Hemley RJ. 2009. Enhancing the mechanical properties of CVD single-crystal diamond. Journal of Physics: Condensed Matter. Issue 36.

Beck P, Goncharov AF, Montoya JA, Struzhkin VV, Militzer B, Hemley RJ, Mao HK. 2009. Response to "Comment on 'Measurements of the thermal diffusivities at high-pressure using a transient heating technique'". Applied Physical Letters. Volume 95, Issue 9.

Zha CS, Krasnicki S, Meng YF, Yan CS, Lai J, Liang Q, Mao HK, Hemley RJ. 2009. Composite chemical vapor deposition diamond anvils for high pressure/high temperature experiments. High Pressure Research. Volume 29, Issue 2.

Liang Q, Yan CS, Meng YF, Lai J, Yu T, Shu H, Krasnicki S, Mao HK, Hemley RJ. Evidence for ultratough single crystal CVD diamond. Phys. Stat. Sol. (forthcoming).

Liang Q, Yan CS, Meng Y, Lai J, Krasnicki S, Yu T, Shu H, Mao HK, Hemley RJ. Ultratough boron-doped CVD single-crystal diamond. Adv. Mat. (submitted).

Beck P, Goncharov AF, Struzhkin VV, Militzer B, Hemley RJ Mao HK. 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, Mao HK, Hemley RJ. High pressure-High temperature Raman spectroscopy of C2 clathrate of H_2-H_2O (to be communicated).