Toshimori Sekine

Shock-Induced Chemistry



Shock Wave and High Pressure Phenomena

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- Initiation and growth of reaction
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- Wave propagation codes
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Applications

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- · Geophysics and planetary science
- Medicine
- · Aerospace and industrial applications
- · Protective materials and structures
- Mining

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ISSN 2197-9529 ISSN 2197-9537 (electronic) Shock Wave and High Pressure Phenomena ISBN 978-981-97-3728-4 ISBN 978-981-97-3729-1 (eBook) https://doi.org/10.1007/978-981-97-3729-1

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Preface

Materials under high pressures change their stabilities, shapes, and properties, and the chemical reactions in mixtures differ from those in the ambient state. Pressure and temperature are thermodynamic parameters, and historically human beings have utilized them to make novel materials to improve the quality of life. Natural phenomena provide a very wide range of pressure from our living environment to the interiors of planets and the collisions of planetary bodies. In our life, we have many benefits from high-pressure science and technology. When we apply high pressure to the gas at room temperature, it changes to liquid and solid depending on the pressure, and it becomes significantly denser. Pressure produces new chemical bonds in the dense state. Diamond is a high-pressure form of carbon. High pressure allows us to explore new materials and new science in physics, chemistry, materials science, planetary science, etc. Therefore, high pressure and high temperature are important variables in basic science and technology.

Recent experimental advances to generate high-pressures as well as high temperatures provide many chances to utilize high-pressure methods. The melting point of most materials generally increases with increasing pressure, and we have extended our ability to investigate solids at high temperatures above their melting points at ambient pressure. Gases under ambient conditions can solidify at high pressure to participate in reactions. Melting behaviors also change with pressure to melt congruently or incongruently. The same change can occur conversely in solidification. In solids, many phase transitions are known, and the structures and properties have been investigated experimentally and theoretically.

Pressure generation methods are classified into static and dynamic compressions. In static compressions, the sample is kept under pressure for long times, and the sample volume is squeezed using multiple anvils to increase the density. The anvil must be hard enough to keep high pressures. Tungsten carbide and diamond are normally used as materials for anvils. The hardest known material is diamond which is widely used to generate pressures in the range of 100s GPa in a small volume. When high temperature is required in static compressions, laser heating or a small surrounding heater is employed to heat up the sample under high pressure. However, it is necessary to calibrate the sample pressure using a standard of pressure when we

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want to determine the pressure. On the other hand, dynamic compressions utilizing inertia to generate and keep high pressures are characterized by pressure profiles that continue for a relatively short time (nanoseconds to microseconds in experiments) depending on the generation method.

Shock chemistry focuses on material synthesis by shock waves that increase pressure and temperature simultaneously and quench the products adiabatically. The process involves rapid compression by shock waves and release of pressure by rarefaction waves. Shock chemistry is associated with wave propagation and depends upon the initial state and the reaction kinetics. However, despite its ubiquitous nature and importance, it is surprising to find that introductory, systematic and comprehensive textbooks of shock-induced chemistry are not currently available to the author's best knowledge.

This book contains 9 chapters. Chapters 1 and 2 give readers the basics of shock chemistry. Chapters 3 and 4 describe the shock chemistry results on hard materials, oxides, nitrides, and other ceramics and minerals, which illustrate syntheses of typical materials by shock compression methods. Chapter 5 is focused on reactions of shock-induced melting and decomposition, mechanochemistry, and sonochemistry. Chapter 6 describes shock reactions of biomolecules in Earth and planetary science systems including shock syntheses of biomolecules related to the origin of life on the Earth. Chapter 7 summarizes shock experiment simulations for shock metamorphism observed in meteorites and impactites that experienced high-pressure and high temperature by hypervelocity meteorites and planetary bodies. Chapter 8 gives recent results on typical Earth and planetary materials under extreme conditions in which the electrons in compounds are partially delocalized by thermal activation. Chapter 9 describes future perspectives on shock chemistry.

I attempted to summarize the current status of shock-induced chemistry based on my interests and updated results. There are many classical references and I apologize to those who have no directly cited references. Although this book will not cover all the issues in shock chemistry, I hope this book provides a basic idea of shock-induced chemistry in condensed matters and some guidance for future shock chemistry. There are many interesting problems to be solved. It is my great pleasure if this book provided some assistance to new participants and researchers who are interested in learning shock chemistry and pushing its boundaries beyond the current state.

Tsukuba, Japan/Shanghai, China January 2023 Toshimori Sekine

Acknowledgments

I wish to express my sincere appreciation to many colleagues and students who have worked together on shock compression studies when I was at the National Institute for Research in Inorganic Materials (NIRIM), the National Institute for Materials Science (NIMS), the California Institute of Technology, Hiroshima University, Osaka University, and the Center for High Pressure Science and Technology Advanced Research (HPSTAR).

When I worked for NIRIM and NIMS, I used a propellant gun and built up a two-stage light gas gun and a laser gun that accelerates a metal mini-flyer to velocities over 10 km/s. Some of the results are summarized in Chaps. 2, 3, 4, 6, and 7. Students from Tsukuba University, Tokyo University, Kobe University, Kyushu University, Tokyo Institute of Technology, Waseda University, Okayama University of Science, and Tohoku University were joined. During the COE project in 1993–2002, approximately ten postdoctorals and JST research fellows were joined together to perform shock compression experiments. We carried out many shock synthesis experiments and characterizations of the recovered samples, especially in ceramic systems. After I shifted to Hiroshima University in 2010, students from Hiroshima University used a propellant gun mostly for shock recovery experiments related to natural impacts described in Chaps. 6 and 7. Collaborative experiments with groups at NIMS, Kumamoto University, and Institute of Fluid Physics were carried out using the gas guns.

Laser shock experiments were initiated as research collaboration at the Institute of Laser Engineering (ILE), Osaka University, before the COE project. Full-scale collaborations at ILE started when I was in the Department of Earth and planetary systems science (DEPSS), Hiroshima University in 2010–2016. Simultaneously a new facility (SACLA) for X-ray-free electron laser (XFEL) was available in 2012, and I joined collaboration research works since then. Chapter 8 is related to the laser shock.

I have joined a staff scientist at HPSTAR after Hiroshima University. Shock chemistry using gas gun and laser shock facilities in China has become a new stage, especially to measure shock temperature and sound velocity. A Korean colleague invited

viii Acknowledgments

me to join shock experiments at a new shock facility at the Pohang Accelerator Laboratory (PAL) where XFEL and laser compression were available to measure in situ X-ray diffractions under compression. In China, lasers such as the Shenguan II (SG II) laser and Shenguan III-prototype (SG III-p) are nanosecond lasers and have been used for laser shock experiments.

The incentive to write this book was provided by several domestic and international lectures and classes at universities and institutes.

Thanks are also due to Yasuyuki Horie who encouraged me to write this book and read the first draft to make comments and suggestions.

Finally, the editorial staffs at Springer helped me to finish up, and without their help, this book could not be brought out.

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Chapter 1 History and Background: Shock Wave, Historical Background, and Compression Process



1

Shock waves deform and compress solid materials at high strain rates. This compression process increases density, temperature, and entropy in the system, and the whole process, including the release process from the compressed state to the original condition, is irreversible thermodynamically. The internal energy increase associated with this compression process increases the temperature, which is expected to enhance chemical reactions. The application of shock waves in solids alters chemical bonds to create novel materials with new bonds and new shapes. The influence of shock waves has been known to be important in various fields including materials science, Earth and planetary science, condensed matter physics, and chemistry under extreme conditions.

As illustrated in Fig. 1.1, there are various applications of shock compression science depending on the strength. Historically, solid samples sealed in a metal container or mixtures of solid samples with an explosive were subjected to shock treatments using hypervelocity impacts or high explosives, and the recovered samples were investigated by various analytical and characterization methods to check the products. The sample amounts were scaled to be on the order of mg to tons of mass depending upon the shock wave generators and recovery systems. This has been the classical method for shock synthesis. Recently, many technical advances have been made to observe in situ deformations and reactions by modern time-resolved methods using electronic equipment (e.g., oscilloscopes), optical methods (fast cameras), and bright, ultrashort-pulse X-ray beams, called X-ray-free electron lasers (XFELs).

Detonation is a complex interplay of chemical reactions and energy transfer that results in a steady shock wave at the front and a release wave at the rear. The rigidity and violence of detonations have not enabled direct observations for a long time, but recent technical developments in hypervelocity impact and laser-driven shocks have provided the capability to observe phenomena directly and can help our further understanding of shock chemistry.