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International Shock-Wave Database Project: Report of the Requirements Workshop

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International Shock-Wave Database Project: Report of the Requirements Workshop

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Abstract

We report on the requirements workshop for a new project, the International Shock-Wave database (ISWdb), which was held October 31 - November 2, 2011, at GSI, Darmstadt, Germany. Participants considered the idea of this database, its structure, technical requirements, content, and principles of operation. This report presents the consensus conclusions from the workshop, key discussion points, and the goals and plan for near-term and intermediate-term development of the ISWdb.

ACKNOWLEDGMENTS

We are grateful to GSI and FAIR managers and staff for their hospitality and help that made this workshop very useful and efficient.

Our special thanks to Prof. Dr. H. Stoker, GSI, Prof. Dr. Th. Stoehlker, GSI, Prof. Dr. B. Sharkov, FAIR, Dr. V. Varentsov, FAIR, B. Schuster-Gruber, GSI.

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EXECUTIVE SUMMARY

We report on a new project, the International Shock-Wave database (ISWdb). This project was discussed during a requirements workshop, October 31 - November 2, 2011, at GSI, Darmstadt, Germany. Participants considered the idea of this database, its structure, technical requirements, content, and principles of operation. This report presents the consensus conclusions from the workshop, key discussion points, and the goals and plan for near-term and intermediate-term development of the ISWdb. The ISWdb will be a successor to an existing shock-wave database, RusBank (<http://www.ficp.ac.ru/rusbank>), which was developed over many years by researchers at Russian Academy of Sciences Institutes and made available via the internet in 1997. The ISWdb will build on the experience with RusBank to achieve our broader current goals. In particular, ISWdb will allow and encourage researchers throughout the technical community to contribute their data and analysis applications, as well as provide comments on data sets or, even, individual data points in the database. Further, the ISWdb will have an on-line bulletin board to foster discussion within the research community.

The main points of consensus from the workshop were:

1. This international database is of interest and of practical use for the shock-wave and high pressure physics communities;
2. Intermediate state information and off-Hugoniot information is important and should be included in ISWdb;
3. Other relevant high pressure and auxiliary data should be included to the database, in the future;
4. Information on the ISWdb needs to be communicated, broadly, to the research community;
5. Operating structure will consist of an Advisory Board, subject-matter expert Moderators to vet submitted data, and the database Project Team.

This brief report is intended to inform the shock-wave research community and interested funding agencies about the project, as its success, ultimately, depends on both of these groups finding sufficient value in the database to use it, contribute to it, and support it. Community involvement will be promoted by presentations at appropriate technical conferences, beginning with the NMH Conference 2012 (<http://www3.imperial.ac.uk/shockphysics/nmh>), through future reports, and through the public bulletin board at the database web site, <http://iswdb.info>.

INTRODUCTION

Shock-wave and related dynamic material response data serve for calibrating, validating, and improving material models over very broad regions of the pressure–temperature–density phase space. Measurements of principal, reflected and porous Hugoniot and determination of release isentrope parameters cover a wide range of the phase diagram. The International Shock-Wave database (ISWdb) project aims to develop a database of experimental results for material response under conditions of shock-wave, other dynamic loadings, and, possibly, static high pressure loading. These data will be supported with selected, related quantities of interest and the meta-data that describes the provenance of the experimental measurements and material models. This database will be made available internationally on the internet, in an interactive form. Our goal is to create a valuable utility for the research community that becomes integral to research projects, both as an archival information resource and as a common, standard repository for experimental results.

The project is supported by the U.S. Department of Energy’s (DOE) Advanced Simulation and Computing (ASC) program’s Russia Science and Technology Program (RS&TP), and is jointly funded by the three DOE National Nuclear Security Administration (NNSA) laboratories: Lawrence Livermore National Laboratory (LLNL); Los Alamos National Laboratory (LANL); Sandia National Laboratory (SNL) – jointly referred to as the Tri-labs. The project receives additional funding, both direct and in-kind, from the Russian Academy of Sciences (RAS). It is being performed by researchers at the Joint Institute for High Temperatures (JIHT) of RAS and the Institute of Problems of Chemical Physics (IPCP) of RAS.

A workshop was recently held for the purpose of identifying requirements, desired features and capabilities of the unclassified ISWdb. The workshop goals included: defining the scope of desired information and functionality of the database; evaluating procedures for reviewing and vetting additions to the database; brainstorming approaches for data collection and engaging the international research community to use and contribute to the database; and identifying candidate members of an advisory board that will help guide the development and operation of the database. The workshop took place in GSI, Darmstadt, Germany, October 31 through November 2, 2011 under patronage of FAIR (<http://www.fair-center.eu/>). The workshop web page is available <http://www.ihed.ras.ru/iswdb2011/>. IPCP RAS has a long-time collaboration with GSI, Darmstadt. Heavy ion interaction with matter overlaps with conditions studied by shock-waves, so many experimental methods and modeling codes of the latter are useful in heavy-ion research. This makes meeting at GSI appropriate.

The workshop united participants from a range of organizations, such as from RAS: Igor V. Lomonosov (IPCP, Chernogolovka), Pavel Levashov (JIHT, Moscow), Dmitry Minakov (JIHT, Moscow); from U.S.A. Department of Energy (DOE) National Laboratories: John Aidun (SNL), Seth Root (SNL), Mukul Kumar (LLNL), Frank Cherne (LANL), Scott Crockett (LANL), Ralph Menikoff (LANL); U.S.A. Universities: Prof. Thomas Sewell, U. Missouri, Columbia; Commissariat à l'énergie atomique et aux énergies alternatives (CEA), France: Olivier Heuze; Germany scientific centers: Boris Sharkov (FAIR), and Rudolf Bock (GSI). They presented oral talks and/or discussed the idea of the database, its structure, content, technical requirements, principles of operation, and subject-matter expertise.

The idea for the ISWdb arises naturally with the progress of Internet and development of corresponding system tools. *“A detailed comparison of new experimental data or new material models with previous work requires that the older data and model parameters be readily*

available. In the past, the research community relied on articles published in conference proceedings and applied journals. Today, almost every researcher has a powerful PC on his desk connected to the internet. Progress in high pressure research would be greatly enhanced if data and model parameters were readily available in electronic form. To meet this need we propose that the APS topical group on Shock Compression in Condensed Matter organize and maintain an electronic database for high pressure research that is accessible, via the internet, to the scientific community.” (R. Menikoff, Y. Horie, Minutes of 2002 Business Meeting of the APS GSCCM. <http://www.shockphysics.org/business.html>). In Russia, we started our project under support of the Russian Foundation for Basic Research in 1997. Now we have an Internet version of database available <http://www.ficp.ac.ru/rusbank/> and <http://www.ihed.ras.ru/rusbank/> (see Appendix 1). The ISWdb will build on the experience with RusBank to achieve our broader current goals. In particular, ISWdb will allow and encourage researchers throughout the technical community to contribute their data and analysis applications, as well as provide comments on data sets or, even, individual data points in the database.

This report presents the consensus conclusions from the workshop, key discussion points, and the goals and plan for near-term and intermediate-term development of the ISWdb.

CONCLUSIONS FROM THE WORKSHOP

In the talks and related discussions, participants formulated the scope and goals of the new international project as follows: ISWdb is (i) a scientific database for free, non-commercial use by the shock-wave community; (ii) free internet access to open published data is granted; (iii) the content includes original shock points and profiles in numerical format with corresponding references. The main points of consensus were the following:

1. This international database is of interest and of practical use for the shock-wave and high pressure physics communities;
2. Intermediate state information and off-Hugoniot information is important and should be included in ISWdb;
3. Other relevant high pressure and auxiliary data should be included to the database, in the future;
4. Information on the ISWdb needs to be communicated, broadly, to the research community;
5. Operating structure will consist of an Advisory Board, subject-matter expert Moderators to vet submitted data, and the database Project Team.

Discussion:

1. The motivation for developing an on-line, interactive database is described above in the Introduction.

i) Data should be vetted by a subject matter expert.

We have a great collection of shock points that have been revised several times, from first original papers to their revisions in compendia like “LASL Shock Hugoniot Data”, ed. by S.P. Marsh. In addition, Igor Lomonosov presented several examples: in early paper by Al’tshuler et al. one can find 7 points in a table and 8 points in a graph and some other tricks.

ii) Data should be presented in a standard format.

We propose to use international system of units to avoid mistakes and confusion in presenting numerical data.

iii) XML format will be used for input.

It is the most suitable format for implementing in the database numerical points, literature references, and text information, describing, for example, the experimental setup. This point is discussed further in the next section.

- iv) Populating the database will start with U_s - u_p data and associated information on the experimental setup.
2. In addition to principle Hugoniot of materials, data on shock compression of porous samples and adiabatic expansion of shocked samples are also of importance for fundamental science and practical interest for developing wide-range EOS. The same motivation remains valid for novel ramp compression data and other experimental information used for developing elastic-plastic and fracture models.
3. In addition to shock-wave data, other useful information would be placed into the database, including normal density, melt and boiling points, melting curves, thermal expansion, acoustic data, specific heat, phonon/elastic moduli, isobaric expansion data and first-principle calculations. These data may also be present as references to other resources.
4. The first release of ISWdb is planned in mid-2012. The response of the technical community is solicited. To advertise ISWdb, this project will be presented in talks at scientific conferences and workshops and on new web site, <http://iswdb.info>. The ISWdb web site will soon have a bulletin board to provide information on ISWdb (project description, vision statement, FAQ, project status) to the technical community and a forum for community input and discussion; also it will have a restricted area for project team and advisory board to communicate.
5. ISWdb management includes an International Advisory Board and Moderators. The advisory board will provide advice, assist with decision making, and represent the interests of the technical community. Its duties, tentatively, are to: monitor the bulletin board as a conduit for communication; provide guidance/advice on scope and direction of ISWdb, including helping with design and implementation decisions; contribute to making other choices of details, e.g., what format for data exchange.

Proposed members of Advisory Board are: one person from each three DOE national laboratories; Prof. Victor Mintsev (IPCP RAS); representatives from Russia Federal Nuclear Centers (RFNC), the French Alternative Energies and Atomic Energy Commission (CEA), the geophysics community; the U.S.A. Department of Defense community, and GSI. The participants in the requirements workshop have agreed to serve as an interim advisory board until permanent members are confirmed.

Moderators' duties, tentatively, are: to review submitted data for completeness and consistency for acceptance into ISWdb; to review papers to accept or reject data for ISWdb; to provide copies of rare papers that a moderator may have. Candidate members are prominent shock-wave physics researchers from government laboratories, universities, and commercial firms.

Project Team members are: principal investigator - I. V. Lomonosov (IPCP&JIHT RAS), principal programmer - P. R. Levashov (JIHT RAS), scientific consultant - V. E. Fortov (JIHT RAS), K. V. Khishchenko (JIHT RAS), D.V.Minakov (JIHT RAS), A. S. Zakharenkov (JIHT RAS), U.S.A. coordinator – J. B. Aidun (SNL). Additionally, one person at each of the three NNSA laboratories acts as “lab champion” for the ISWdb to represent their respective laboratory

in project planning discussions and to communicate information about the ISWdb back to their home institution.

Early in 2012 the project team will be contacting individuals from the research community to invite them to serve as advisory board members or moderators.

PLANNED DATABASE STRUCTURE

The ISWdb is a complex system that is intended to be a practical tool for a wide community of scientists. Therefore the structure of the ISWdb includes both technical and organizational requirements.

The hardware requirements for the ISWdb operation are moderate. We plan to mirror the site on two standard Linux servers (one in Russia and one in the United States). Well-tested, robust, open-source software will be installed on each server, including Apache Web server as an internet server and PostgreSQL as a database server.

All the data will be stored into the SQL-database. All experimental points will have error bars or error estimates, as far as possible. The intermediate format for data editing and exchange will be XML. This allows one to keep any type of information, including shock-wave profiles, meta-data, comments, and references. Both users and Moderators will be able to tag data points to add comments to them.

All the data in the database will be taken from published or otherwise referenceable, open sources so that any experimental point in the database will have a bibliographic reference. All these references will be organized into a bibliographic database with the possibility to represent references in different formats, including BibTeX. Also there will be a hyperlink to the original publication on the Internet, if possible.

A very important feature of the database is the ability to search necessary data by different criteria. A search function will be worked out and implemented in the ISWdb to allow one to look for experimental points by type, year, reference, substance, chemical formula, comment, and, probably, other criteria.

The ISWdb will have rich capabilities to represent experimental data, in particular, in tabular and textual forms. The tabular representation will allow sorting data by columns. Different units can be used in data output; a user will be able to download several datasets at once.

Also, a capability will be provided to output/download data as graphs with rich formatting capabilities. In particular, a user will be able to change axes limits, values, scales; enable/disable curves or data points; compare experimental data with available models and approximations. Several graphical formats will be provided for download, both raster and vector, including SVG and EPS. Additionally, we will post a guide for users who may want to supply plug-in analyses, models, or other applications to extend the functionality of the ISWdb.

The registration to access the ISWdb will be free. All members of Advisory Board and Moderators will have special accounts with capabilities to edit experimental and other information in the ISWdb. Administrators on the project team will be responsible for the overall operation of the ISWdb, including software updates, backups, registration of users with special rights and other administrative obligations.

We plan to add links to existing internet-based projects in shock wave physics, in particular, to HED (High Explosives database) at LANL, to MIDAS (Material Implementation, Database, and Analysis Source) at LLNL.

CONCLUSIONS

A workshop to develop requirements for the International Shock Wave database took place at GSI, Darmstadt, Germany from October 31 to November 2, 2011. Participants from USA, Russia, France and Germany discussed the idea of the new project - an open, unclassified, searchable repository of shock-wave physics data for free, non-commercial use. The discussions included technical details of the database structure, format of input data, requirements for data quality, demands on internet and database servers, and other related challenges. Subsequent discussion defined types of shock data to be implemented in the database, demands to the database interface and service functions, possible candidates for the Advisory board and Moderators of experimental data entry. Consensus conclusions are that this international database is of interest and of practical importance for the shock-wave and high-pressure physics communities. An overview of the database, its structure, technical requirements, content, principles of operation and expertise of information are presented in this report. The first release of ISWdb is planned in mid-2012.

The response of community is solicited, both in response to presentations that will be made at upcoming technical conferences and through the bulletin board that will soon be added to the ISWdb site (<http://iswdb.info>). This bulletin board will be used to provide the technical community information on ISWdb and provide a forum for community input and discussion. In upcoming conference talks and future reports we will aim to provide illustrative examples of the variety of data that can be included, formats for the data, and the data submission process. Additionally, the developing membership, duties, and actions of the Advisory Board and Moderators will be reported on in the bulletin board.

Appendices

Appendix 1 – Background and Perspective

IPCP and JIHT currently maintain an online shock-wave database (<http://www.ficp.ac.ru/rusbank>). Data collection and selection was begun by L. Al'tshuler and A. Bushman from 1975 to 1981. A. Bushman continued this work until 1993, being joined by I. Lomonosov in 1984. I. Lomonosov and K. Khishchenko continued data selection from 1993 to 1997. In 1997 I. Lomonosov, K. Khishchenko, P. Levashov, and I. Lomov produced the first version of the database as an internet-enabled utility. It contains data from available Russian experiments, the LLNL and LANL compendia, and journals, proceedings and reprints, as well. Further work on the database was funded by three Russian Foundation for Basic Research (RFBR) grants between 1997 and 2007. In this period new types of data and new functionalities were added. Direct investments from Russia Federation grants and others funds in the shock-wave database from 1997 to 2007 total \$200,000. The data collection and selection effort from 1975 to 1997 comprised about 30 man-years of work; a figure that much more accurately reflects the real value and investment than does the dollar amount of historic funding.

Independently, in 2002 Ralph Menikoff (LANL) and Yasuyuki Horie (then at LANL) proposed creation of an EOS database to the Shock Compression of Condensed Matter (SCCM) topical group of the American Physical Society (APS). That proposal is available on the SCCM web site under 2002 "Proposal for a Shock Physics Database" (<http://www.shockphysics.org/EOSproposal.pdf>) Also see the end of the minutes of the 2002 business meeting (<http://www.shockphysics.org/business.html>) for a note about Horie's comments on a database.

A few years later, I. Lomonosov initiated discussions with J. Aidun on his idea to update and expand the RusBank shockwave database. At the 2007 SCCM technical meeting, the idea was presented to prominent researchers from the shock-wave physics communities at each of the three NNSA labs, and discussed at the business meeting. Attendees included R. Menikoff and Y. Horie. I. Lomonosov and P. Levashov briefed the ISWdb idea to Dimitri Kusnesov (NNSA) and members of the Russia S&T programs at SNL and LANL at the May 2008 meeting on New Models and Hydrocodes for Shock Wave Processes. In July 2011, J. Aidun and J. Kamm, who had become manager of the RS&TP at SNL, provided initial NNSA funding for the ISWdb project. More recently, R. Menikoff and C. Scovel developed the unclassified High Explosives Database (HED) at LANL (<https://hed.lanl.gov/>). That database is focused on experimental, rate-dependent data on the response of reactive materials to shock-wave loading. At the requirements workshop Menikoff provided the benefit of several of the considerations that went into developing the HED and some lessons gained from the experience of constructing it.

Appendix 2 – Workshop Participants

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Set Root*, Ph.D., sroot@sandia.gov

University of Missouri, Columbia
Prof. Thomas Sewell, sewellt@missouri.edu

* Lab champion for ISWdb



Figure 1. Workshop Participants

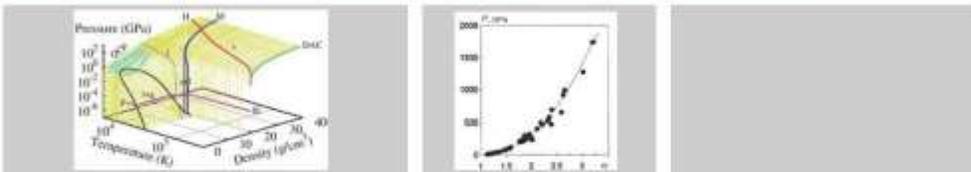
From left to right: I. Lomonosov, R. Menikoff, D. Minakov, T. Sewell, S. Crockett, S. Root, J. Aidun, O. Heuze, F. Cherne, M. Kumar, and P. Levashov

Appendix 3 – Workshop Presentations

Participants presented following talks at ISWdb workshop:

- ISWdb Requirements Workshop Background & Goals (J. B. Aidun)
- International Shock-Wave Database: Preserving and Sharing of Forgotten Shock-Wave Data (I. Lomonosov)
- Principles and Technical Aspects of the ISWdb (P. Levashov)
- International Shock-Wave Database: Sandia Perspective (S. Root)
- Summary of Current Shock and Detonation Physics Research at Los Alamos National Laboratory (F. Cherne)
- The Perspective from LLNL (M. Kumar)
- Database Design Issues (R. Menikoff)
- Constraining EOS to experimental and theoretical data (S. Crockett)

These reports covered all aspects of ISWdb: details of content; format of data; technical aspects; messages from EOS developers and from experimentalists dealing with extreme pressures, detonation and inelastic deformation, fracture and spall. Positive and stimulating, wide ranging “round table” discussions accompanied and followed the presentations. The presentation slides are included below.



ISWdb Requirements Workshop

Background & Goals

John B. Aidun

U.S. Coordinator of ISWdb project

The ISWdb Idea.



- International Shockwave Database idea:
 - ICP-JIHT Database –
 - Data collection and selection was begun by L. Al'tshuler and A. Bushman from 1975 to 1981.
 - Bushman continued this work until 1993.
 - Bushman was joined by Lomonosov in 1984.
 - Lomonosov and K. Khishchenko continued data selection from 1993 to 1997.
 - In 1997 Lomonosov, Khishchenko, P. Levashov, and I. Lomov produced the first version of the database as an internet-enabled utility at <http://www.ficp.ac.ru/rusbank>
 - Ralph Menikoff & Yuki Horie wrote an EOS database proposal in 2002
 - Discussed at TCG SCCM business meeting at March 2002 APS meeting.
 - See <http://www.shockphysics.org/business.html> for proposal and minutes
 - Lomonosov began discussing idea of ISWdb with Aidun by 2007
 - Discussed at SCCM07 in Hawaii.
 - Draft proposal and presentation at New Methods 2008 (Estoril)
 - First funding for JIHT work on ISWdb began in 2011.

Menikoff-Horie 2002 database proposal

(Y. Horie told me about this proposal in March 2008)

1. Database available through the web and available to all researchers.
2. As an electronic database, can continually add new data and correct errors.
3. Database should include:
 - experimental data;
 - EOS models with fitting parameters for specific materials;
 - Synthetic data from numerical "experiments" such as molecular dynamics or Monte Carlo simulations.
4. Researchers should contribute data, as well as use it.

[Menikoff: personal comm.]

3

Menikoff-Horie 2002 proposal - Benefits

- Having material data readily accessible encourages comparison between different experimental data sets, and between models and experiments.
- Results of a simulation are no better than the data that goes into them. EOS model parameters are key input data.
- By referring to a specific material in a database, the model along with parameters would be fully specified without the need to duplicate the description of model in every paper.
- Validation of models is an important issue for doing good science.
 - It would be a great advantage to divide up this time-consuming work by having the careful work of one researcher available to others
 - A common database would facilitate and encourage such cooperation.

4

Menikoff-Horie 2002 proposal - Steps



Steps anticipated by Menikoff:

1. Decide what information the database should include;
2. Select a format for exchange of electronic information;
3. Devise protocols for access to the database
 - e.g., to maintain scientific integrity, researchers should submit contributions to a “moderator”.
4. Set up a web server
 - Requires finding a funding sponsor.

6

ISWdb Goals.



- International Shockwave Database:
 - Developing a database on thermodynamic and mechanical properties of materials under conditions of shock wave and other dynamic loadings
 - selected related quantities of interest
 - the meta-data that describes the provenance of the experimental measurements and material models;
 - Make available internationally on the internet, in an interactive form.

5

Workshop Goals.



- Workshop:
 - defining the scope of desired information and functionality of the database;
 - evaluating procedures for reviewing and vetting additions to the database;
 - brainstorming approaches for data collection and engaging the international research community to use and contribute to the database;
 - anticipating challenges and obstacles to success;
 - identifying candidate members of a steering committee that will help guide the development and operation of the database.

6

ISWdb Challenges.



- Technical
 - How to gather data from published articles?
 - Copyright issues?
 - How to set up a mirror site in U.S.A?
 - Expanding visualization capabilities.
 - Optimize the GUI for ease of use.
- Social
 - Will need to iterate with community getting input/feedback and modifying the database
- Programmatic
 - How to manage and maintain the database over the long term?

7

Desired Features follow



10

ISWdb – a few desired features.



- **Technical**
 - A range of data types – useful for wide-range EOS development
 - DFT cold curves
 - DAC hydrostats
 - Isobaric expansion
 - CTE
 - DFT-MD for critical point data
 - Include raw data, as well as density normalized data
 - Include capability to scale to a chosen density
 - Include reported uncertainties
 - Include metadata
 - Report how data was captured
 - Typed in from a table; scanned; digitized.
 - Make numerical manipulations transparent to user
 - e.g., computing ρ & D when only P & u are reported; recentering Hugoniot
 - Make analyses downloadable
 - Permit users to conduct analyses off-line.

8

ISWdb – a few desired features.



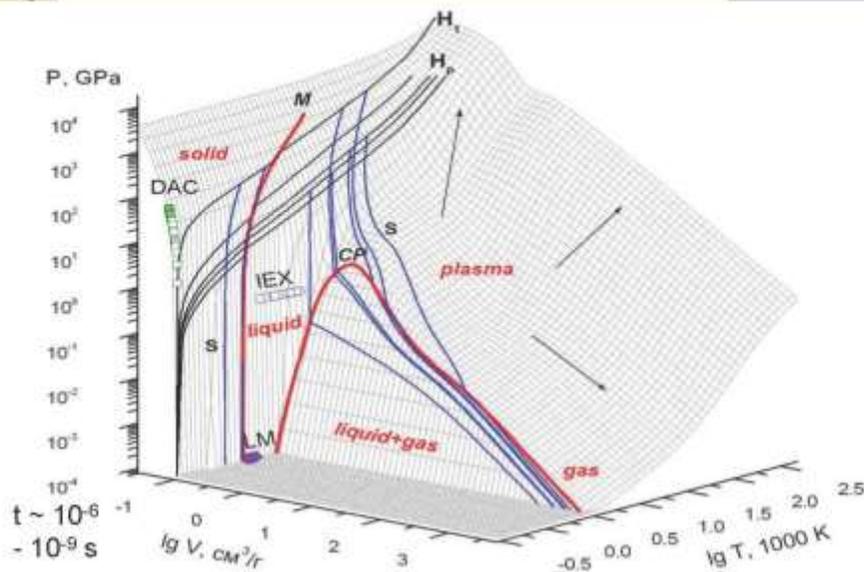
- Social
 - Do we need a more inclusive name?
 - ISHPdb, perhaps?
 - Need a capability for users to leave comments and provide feedback
 - A wiki page or Trac site, perhaps?
 - Blog site or Message Board?
 - Other communities that we need to engage
 - ISP GB (Wm. Proud)
 - AWE
 - Japan
 - China
 - Static High Pressure community
 - Geophysics community
 - AIRAPT

International Shock-Wave Database: Preserving and Sharing of Forgotten Shock-Wave Data

I.V.Lomonosov
IPCP RAS, 142432 Chernogolovka, RUSSIA

- ❖ Preamble
- ❖ Shock-wave data for Al
- ❖ Objectives
- ❖ Motivation
- ❖ Scientific & technical description
- ❖ Potential users
- ❖ Previous funding & experience
- ❖ What's new
- ❖ Key stuff

Preamble: shock waves



Preamble: shock waves

Shock-wave data summary:

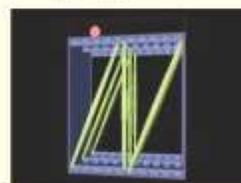
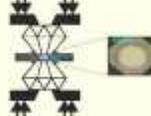
- unique physical nature
- 9 orders – pressure, 4 – density
- high fidelity
- main info for models calibration
- standard for high pressure science
- importance for XXI key problems:
 - # space (impact craters, space debris)
 - # energy (inertial confinement, pulsed power)



heavy ion beam



Diamond Anvil Cell



3

Shock-wave data and Al EOS

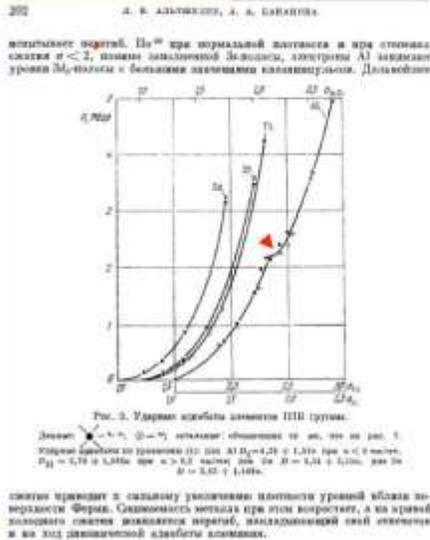
- set of revised shock-wave data
- Al – material for Z
- Al – reference metal for WDM research
- multi-phase EOS for Al – old data
SESAME 78, Holian 86, Kerley 87, Bushman 88
- phase transition in Al at 2 Mbar?
- previous shock data
- Z-data:
 - # shock adiabat to 5 Mbar
 - # $s=\text{const}$ to 3 Mbar
 - # release isentropes for liquid Al

4

Phase transition at 200 GPa (Altshuler & Bakanova, Sov.Phys.-Usp., 1968)



Лев Витальевич Алтшулер
(9.11.1913 - 23.12.2003)



Phase transition at ~200 GPa:

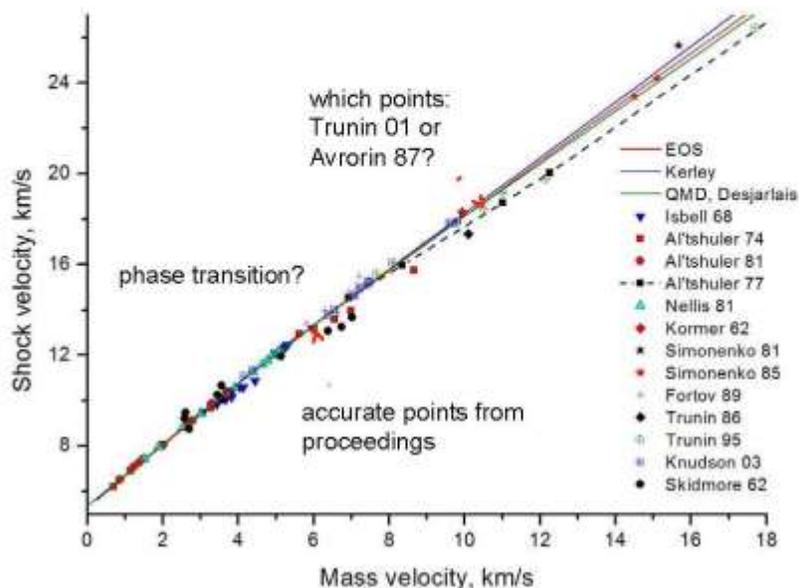
pro

- Gandelman Sov.Phys.-Usp 1970
- McMahan PRB 1983
- Cohen PRB 1983
- Lam PRB 1991
- Boettger PRB 1996
- Sinko JPh:Cond. Matt. 2002
- Akahama (DAC) PRL 2006
- Sinko 2007

contra

- Shock waves 1962-2005
 - Ruoff (DAC) PRL 1994
 - Davis (s=const) JAP 2006
- (no dramatic anomalies)*

Al shock adiabat: Z region



Al phase diagram

accurate points from
proceedings

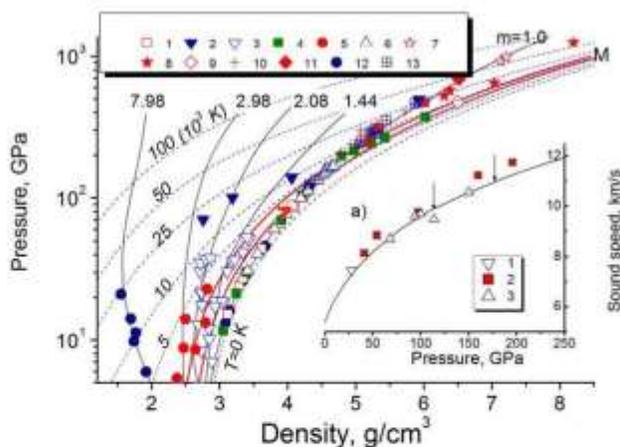


Fig. 9. Phase diagram of aluminum at high pressures. Nomenclature: lines—EOS calculations, T—isotherms, M—melting region, m —shock adiabat of porous samples ($m = \rho_0/\rho_{00}$ —porosity); points—experimental data, 1—Al'tshuler *et al.* (1981), 2—Kormer *et al.* (1962), 3—van Thiel (1977); 4—Al'tshuler *et al.* (1960a); Al'tshuler & Chekin (1984), 5—Bakanova *et al.* (1974), 6—Mitchell & Nellis (1981), 7—Simonenko *et al.* (1985), 8—revision Trunin *et al.* (2001) of original data Avrorin *et al.* (1987), 9—Trunin (1986), 10—Glushak *et al.* (1989), 11—Trunin *et al.* (1995a), 12—Trunin *et al.* (2001), 13—Knudson *et al.* (2003). a) Sound speed in shocked aluminum. Line—EOS, points—experiment, 1—Neal (1975), 2—Al'tshuler *et al.* (1960b), 3—McQueen *et al.* (1984), arrows indicate the melting region.

Al shock data

- numerous revisions:
 - papers – High Vel. Imp. Phen. – LASL
- important data – in conference proceedings
- influence from personal point of view
- cited data - for Al alloy 2024

- Al'tshuler's paper 1960-th – 7 points in table, 8 – in graph

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Shock Hugoniot data

Elements

Select substance: Press: to get the desired substance.

Aluminum, Al

$R_0 = 2.712 \text{ g/cc}$

[Graph](#) | [Plain text](#)

m	U , km/s	D , km/s	P , GPa	R/R_0	R , g/cc	$E - E_0$, kJ/g	Remarks	References
1.000	2.8	5.33	69.330	1.442	3.9116	3.920		1. I. V. Al'tshuler et al. 1950
	3.69	10.39	103.976	1.551	4.2056	6.808		
	4.62	12.94	197.224	1.768	4.7942	15.792		
1.000	1.92	7.92	41.240	1.320	3.5798	1.843		2. I. V. Al'tshuler et al. 1960
	2.36	8.52	54.531	1.383	3.7510	2.785		
	2.8	9.13	69.330	1.442	3.9116	3.920		
	3.54	10.2	97.925	1.532	4.1535	6.266		
	3.77	10.5	107.355	1.560	4.2312	7.106		
	4.89	12	160.442	1.697	4.6033	12.352		
	5.59	12.9	195.565	1.765	4.7859	15.024		
1.000	1.72	7.72	36.031	1.287	3.4894	1.479		3. I. V. Al'tshuler and A. P. Petrus 1961
1.000	9.935	18.31	493.340	2.186	5.9292	49.352		4. S. B. Konner et al. 1962
1.435	6.27	11.74	139.123	1.496	4.0564	19.656		4. S. B. Konner et al. 1962
2.086	6.76	11.42	100.159	1.175	3.1858	22.849		4. S. B. Konner et al. 1962

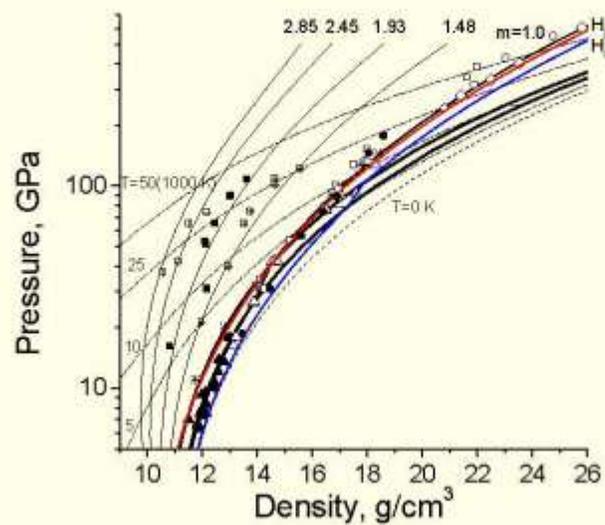
10

Shock data for porous material (Bi)

w	U , km/s	D , km/s	P , GPa	E/E_0	R , g/cc	$E - E_0$, kJ/g	Remarks	References
	6.5	10.6	6.75	1.20	2.576	25.5566		41.125
1.486	1.19	2.66	20.955	1.218	11.9790	0.708		23. B. I. Ginzhak et al. 1989
	1.71	3.5	39.621	1.316	12.9441	1.462		
	2.24	4.39	65.099	1.374	13.5171	2.509		
	2.42	4.67	74.815	1.397	13.7402	2.928		
	2.89	5.27	100.825	1.490	14.6586	4.176		
	2.99	5.46	108.074	1.488	14.6337	4.470		
	3.24	5.64	120.971	1.582	15.5570	5.249		
1.929	1.29	2.44	16.053	1.100	10.8209	0.832		23. B. I. Ginzhak et al. 1989
	1.87	3.22	30.709	1.237	12.1644	1.748		
	2.44	4.22	52.514	1.229	12.0910	2.977		
	2.74	4.64	64.839	1.266	12.4547	3.754		
	3.26	5.35	88.949	1.327	13.0550	5.314		
	3.63	5.8	107.375	1.386	13.6313	6.588		
1.967	2.46	4.18	51.414	1.235	12.1512	3.026		23. B. I. Ginzhak et al. 1989
	3.3	5.36	88.440	1.323	13.0097	5.443		
2.459	2.6	4.06	42.224	1.131	11.1233	3.380		23. B. I. Ginzhak et al. 1989
	3.51	5.23	73.429	1.237	12.1628	6.160		
2.859	2.7	4	37.152	1.076	10.5846	3.645		23. B. I. Ginzhak et al. 1989

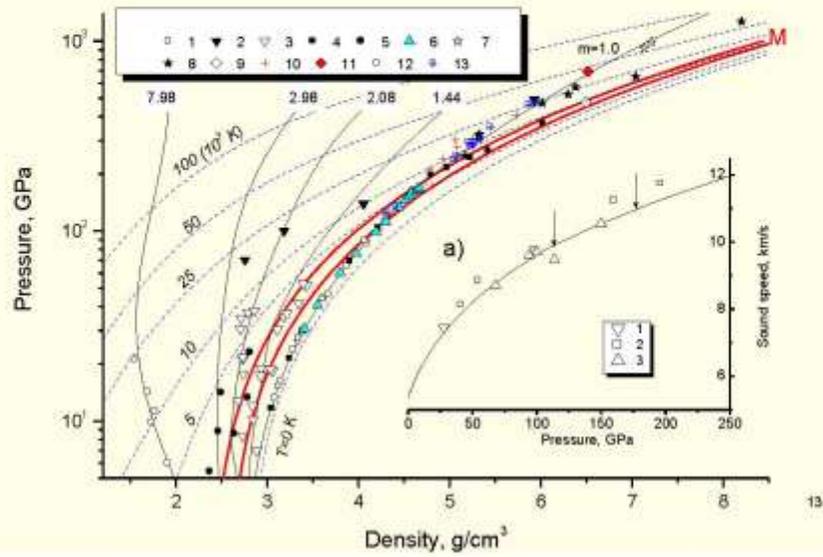
11

Shock Hugoniots for solid, porous, cooled and liquid metal (Bi)

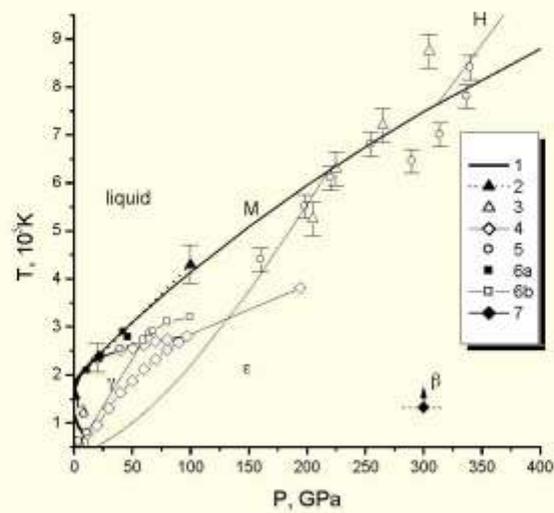


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Sound speed in shocked metal (Al)



T data for shocked metal (Fe)



Release isentropes

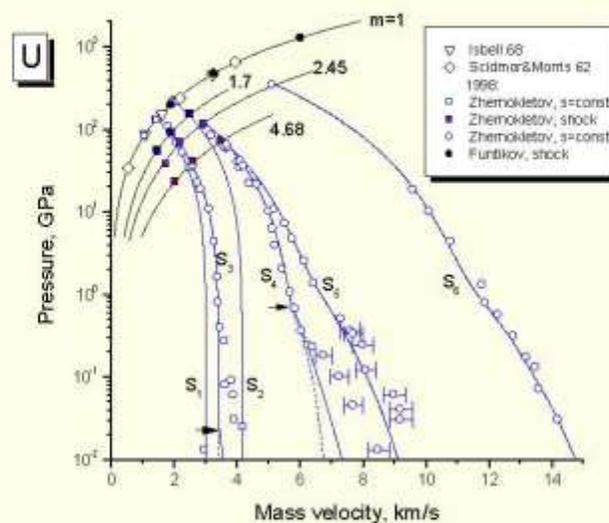
Uranium, U

$R_0 = 19.04 \text{ g/cc}$

[Graph](#) [Plain text](#)

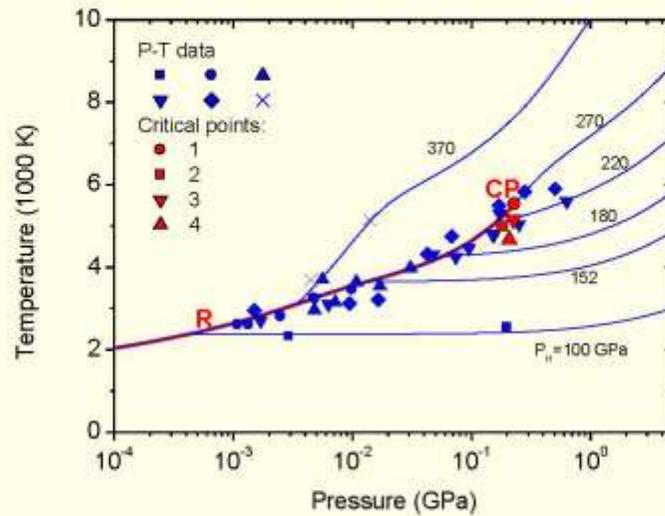
m	$U_0, \text{ km/s}$	$P_0, \text{ GPa}$	$U, \text{ km/s}$	$P, \text{ GPa}$	Remarks	References
1.006	6.78	1510.79	16.3	0.38		1. Ph. de Beaussonnet and J. Leygnon 1970
1.018	1.46	129	2.98	0.013		2. M. V. Zhernokletov 1998
	1.97	208	4.19	0.025		
1.660	1.9	90.5	1.94	87.3		2. M. V. Zhernokletov 1998
			2.1	67.1		
			2.27	51.7		
			2.51	33.4		
			2.6	35.7		
			2.76	22		
			2.85	18.5		
			3.12	10.7		
			3.29	4.3		
			3.38	1.6		
			3.4	0.79		
			3.47	0.39		
			3.6	0.27		
			3.63	0.08		

Release isentropes (U)



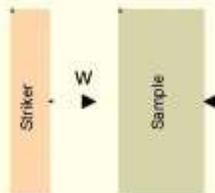
16

Release isentropes – T data (Pb)



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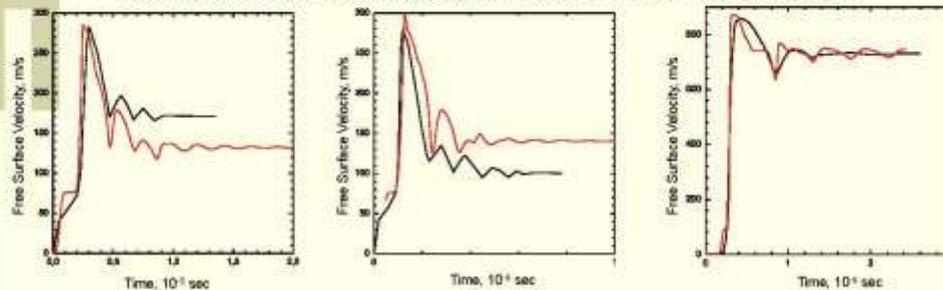
Free surface velocity profiles: calibrating rheological models



Experiments parameters *

Exp#	Plate material	h_{sample} mm	h_{striker} mm	w , m/s
1	Al	9.6	0.1	660
2	Al	4.4	0.2	660
3	Mg	10.0	2.0	700

Experimentally measured (black) and computed (red) free surface mass velocity profiles



Shock data: summary

- different sources: papers, proceedings, reports
- shock adiabats:
 - solid, porous, cooled, heated material
- sound speed in shocked material
- release isentropes
- any temperature data
- free-surface-velocity profiles

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Objectives

- searching of data from papers, proceedings, reports
- critical analysis
- developing of Internet data base on thermodynamic and mechanic properties
- online access to experimental data on shock compression, release expansion, measurements of the sound speed in shocked material, and time-dependent free-surface-velocity profiles
- 2 mirror servers in Russia & USA

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Motivation

- XXI century – industry of knowledges
- main source of information: Internet
- not everything is available
- shock-wave compendiums (LLNL, LASL, ICP, Sarov) are not full
- NIST data bases are local & no SW-data
- in practice researchers needs original experimental points + reference
- shock-wave community needs internet data base with original data

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Scientific&Technical Description

- data collecting & recognizing & digitizing
- system software: FSF products, UNIX, Apach, PHP, PostgreSQL, Perl
- material groups = LASL compendium
- numerical points w references for shock adiabats, release isentropes & free surface velocity profiles
- output: *html, ascii, jpg*
- scalability
- additional parts: www-board, tutorial, help, links, people

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Previous experience

- 1975–1981: data selection by L.Al'tshuler, A.Bushman
- Till 1993: A.Bushman, I.Lomonosov (from 1984)
- 1993-1997: I.Lomonosov, K.Khishchenko
- 1997: first version of Internet database, I.Lomonosov, K.Khishchenko, P.Levashov, I.Lomov
- 1997-2007: 3 RFBR grants to extend & support this data base, <http://www.ficp.ac.ru/rusbank>
 - # new types of data
 - # new possibilities

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Previous funding

- RFBR support from 1997: 10 years, ~15,000\$/year = 150,000\$
- Presidium RAS Scientific Programs from 2002: 5 years, ~2000\$/year=10,000\$ (hardware)
- Total direct investments from 1997: **200,000\$**
- Collecting data from 1975 to 1997: ~30 man*years

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What's new

- **system tools:** ~50000 lines of code will be completely rewritten
- extension of information (experimental methods, accuracy, ...)
- new data: 3 labs reports, conference proceedings, ...
- data expertise by community (R.Menikoff's idea)
- better scalability & reliability

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Key stuff

- Prof. I.V.Lomonosov, IPCP RAS - principal investigator
- Prof., academician V.E.Fortov, JIHT RAS – scientific consultant
- Dr. K.V.Khishchenko, JIHT RAS – investigator
- Dr. P.R.Levashov, JIHT RAS – investigator, principal programmer
- Other programmers & technicians: 6 persons, IPCP RAS, JIHT RAS

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Principles and Technical Aspects of the ISWdb

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1st Workshop on International Shock-Wave Database
Oct 31 – Nov 2 2011, GSI Darmstadt, Germany

Outline

- Principles of Web technologies
- Requirements to ISWdb
- Technical aspects of the existing prototype
- What should be improved
- First steps

Principles of Web Technologies



HTTP Protocol

- HyperText Transfer Protocol, Tim Berners-Lee group, 1991
- Text stateless protocol (connection is closed after response)

Request from the client to get the file `index.html` from `www.example.com`:

```
GET /index.html HTTP/1.1<CR><LF>
Host: www.example.com<CR><LF>
<CR><LF>
```

Response from the web-server:

```
HTTP/1.1 200 OK
Date: Mon, 23 May 2005 22:38:34 GMT
Server: Apache/1.3.3.7 (Unix) (Red-Hat/Linux)
Last-Modified: Wed, 08 Jan 2003 23:11:55 GMT
Etag: "3f80f-1b6-3e1cb03b"
Accept-Ranges: bytes
Content-Length: 438
Connection: close
Content-Type: text/html; charset=UTF-8
<CR><LF>
...
```

headers

Web-server

Media type and encoding

Text of the page

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HTML language

- Created by Tim Berners-Lee in 1990
- HTML (HyperText Markup Language) uses tags to create headings, paragraphs, lists, links, quotes, tables etc. and also to insert images and objects

Example:

```
<!DOCTYPE html>  
<html>  
<body>  
  <h1>Hello World!</h1>  
</body>  
</html>
```

Document type declaration

First-level heading

Result:

Hello World!



HTML elements are the basic building-blocks of webpages

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Generation of Web-Pages (CGI)

- The web-pages written in HTML can be stored into the files with extensions .htm or .html
- However, the web-page can be also generated on the server by some program called by the web-server
- This technology is called the Common Gateway interface (CGI) and the program – CGI-script
- CGI-script is relatively easy to write as both HTTP and HTML are textual; any language with input/output capabilities can be used (FORTRAN, BASIC, Pascal, C, etc.)
- However interpreted languages are preferable as you don't need to recompile the CGI-script after every small change: Perl, Python, Ruby, PHP, etc.
- Web browsers can send parameters to the CGI-script thus changing the generated web-page



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Scripting Languages for Web

- Perl 5 is a highly capable, feature-rich programming language with over 23 years of development. Perl 5 runs on over 100 platforms from portables to mainframes and is suitable for both rapid prototyping and large scale development projects.
- PHP is a widely-used general-purpose scripting language that is especially suited for Web development and can be embedded into HTML.
- Python is a remarkably powerful dynamic programming language that is used in a wide variety of application domains
- Java is a programming language and computing platform; Java runs on more than 850 million personal computers worldwide. JSP is the technology for writing Web-applications using Java



There are many other technologies:
ASP, CSP, ColdFusion, Groovy, Lotus Domino, Real Studio,
Ruby, Smalltalk, Websphere, .NET, ...



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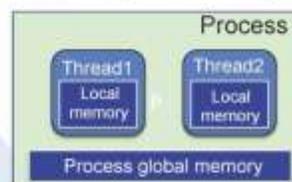
Generation of Web-pages



Every request from the web-browser originates the new process
This process, in turn, calls the CGI-script
After the response both processes are destroyed:
the workload on the server is significant!

Solutions:

- Launch 1 CGI-script and don't destroy it (**FastCGI**) – Perl, PHP, Python, etc., requires specially designed scripts
- Launch the CGI-script inside the Web-server process (using modules) – Perl, PHP, Python, etc., Web-server should support this technology
- Launch a new thread inside an existing Web-server process (JSP and many other commercial solutions)



- Each process has its own memory
- Thread is created **inside** the process and can share memory with other threads
- Using thread can significantly reduce the consumption of memory



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Database SQL Server

Relational model: relations (tables) and constrains

Relational databases are managed by the relational database management systems (**RDBMS**)

SQL (structured query language) allows one to manage data in RDBMS

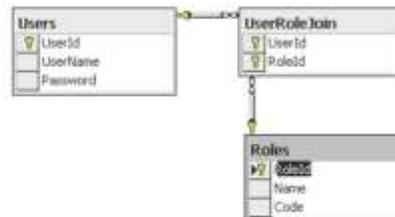
Example of SQL query and response:

```
mysql> select * from roles;
```

roleid	name	code
1	Administrator	adm
2	Editor	edt
3	User	usr

3 rows in set (0.00 sec)

Many-to-many relationship



RDBMS: DB2, Oracle, Microsoft SQL Server, PostgreSQL, MySQL, etc.



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Additional Web Technologies

- JavaScript is a client-side language. It interprets by client applications (mostly Web-browsers). This allows one to change the view of the Web-page without any requests to the server
- CSS (Cascading style sheets) is a style sheet language used to describe the presentation semantics (the look and formatting) of a document written in a markup language (HTML)
- **AJAX (Asynchronous JavaScript and XML)** is a group of interrelated web development methods used on the client-side to create asynchronous web applications. With Ajax, web applications can send data to, and retrieve data from, a server **asynchronously (in the background)** without interfering with the display and behavior of the existing page. [Google Maps](#), [Gmail](#), [Google Documents](#) and many other applications are based on the AJAX technology.



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Desktop application vs. Web-Application

Desktop application is usually run by a single user. It needs

- Computer with operating system

Web-application is run by multiple users. So it needs much more:

- Server-side code (runs on the server side)
- Client-side code (runs on the client side)
- Web-server (to get requests and run the server-side code)
- Web-client (browser, to send requests, interpret responses from the Web-server and run the client-side code)
- Network connection (to establish connection between the server and client)
- Some storage for collective access (the database is very convenient for this purpose)



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Representation of Graphs via the Web

- Static pictures can be requested and represented directly by browsers
- Different raster formats are supported (gif, jpeg, png)
- Some vector formats such as SVG
- Dynamic picture should be somehow generated
 - on the client side (by the use of Java-applet or JavaScript)
 - on the server side using external applications such as gnuplot, GLE, etc.
 - on the server side by means of the scripting language modules – Perl, PHP, etc.)



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Using external modules in Web-applications

- External modules such as equations of state can be written in other programming languages (FORTRAN, C++, etc.)
- They can be even run under different operating systems
- To make it possible the external module should be a filter, e.g. it takes all the data from the standard input and writes the data to the standard output
- Thus the CGI-script running on the server side can communicate with the module through the input and output files (redirection)
- This technology can be used for running any external programs



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Minimal requirements to ISWdb

- Data representation in tabular and textual form (different formats)
- Data representation in graphical form with the possibility to adjust graph parameters (axes, scales, physical properties etc.)
- Possibility to add end edit information in the database
- Management of the database



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Additional requirements to ISWdb

- Experimental data approximation with simple empirical dependencies
- Experimental data approximation with equations of state
- Equation-of-state calculations
- Self-similar simulation of shock-wave experiments
- 1D hydrodynamic simulation of shock-wave profiles
- ...



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Hardware requirements

- 1 processor Intel Xeon, 4 cores, 64-bit architecture, CPU frequency not less than 2.5 GHz;
Moderate computational resources, simple and robust algorithms
- Not less than 4 Gb RAM;
The amount of experimental data is moderate; usage of thread-safe modules and applications may reduce the consumption of memory
- 300 Gb disk space and access to NAS;
300 Gb is a standard size of disk drive in modern servers, access to NAS is desirable for making backups
- 2 network (Ethernet) interfaces, 1 Gb/s
1 interface is for Internet connection (sufficient bandwidth for the current purposes), the other may be used for the external connection to the server
- For 1D hydrodynamic calculations the requirements to CPU and RAM may be toughen up



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Server Software Requirements

- **Debian Linux;**
Very stable, free, supported by a vast community, contains all necessary packages
- **Apache http-server;**
The most popular Web-server in the world; very flexible, works on almost every platform, contains support for many technologies, including FastCGI, modules, threads, scripting languages etc.
- **PostgreSQL database server;**
Very stable, free, supports all necessary technologies including replication of data
- **PHP scripting language**
One of the most popular Web-scripting languages in the world, dynamic, object-oriented, includes many technologies; access to databases, graphics, archives, many data formats (more than 100 modules)

Alternative:

- **Apache Tomcat server;**
Support servlets and JSP, free.
- **J2EE SDK**
Contains all necessary modules for creation Web-applications with Java, free



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List of Modules of the ISWdb

1. **Module for representation of data in a textual form.**
This module is intended to reproduce all types of experimental and calculated data in textual form for subsequent treatment by local programs.
2. **Module for representation of data in a tabular form.**
The tabular form is a convenient and widespread way of representation of experimental data. Additional possibilities will be provided such as the choice of columns and sorting by a column.
3. **Module for representation of data in graphical form.**
All types of experimental data will be represented in a graphical form with the possibility to control the graph parameters. Among experimental data other information can be placed on a graph such as approximations and calculations by simple EOS models.
4. **Module for calculation of thermodynamic parameters and also different thermodynamic curves by simple EOS models.**
This module can be used in the previous one and also separately, as a tool for making EOS calculations.



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List of Modules of the ISWdb (cont.)

5. Administration module (authorization, user management, database control, import and export of data).
This module will be used by the administrators and is intended to simplify the maintenance of the ISWDB.
6. Data editing module (addition or editing all the data in the database).
This module will be used by users with special permissions to add and modify experimental data in the database.



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SHOCK WAVE DATABASE

URL: <http://teos.ficp.ac.ru/rusbank/>
<http://www.ihed.ras.ru/rusbank/>

- 6 types of experiments
- About 21000 registrations for more than 500 substances
- 4 types of shock-wave data approximations
- 3 types of caloric EOS
- Access via the Internet using common browsers
- Graphical representation of all data
- EOS calculations (shock Hugoniots, release isentropes, isobars, isochors, cold curves etc.) with graphical representation
- Modeling of typical shock-wave experiments
- 1D hydrodynamic simulation of shock-wave experiments



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Search by Substance

Search substances

The number of results: The number of pages:

Type can iterative regular expression for substance name (empty expression - all substances):

Note: see definitions below the table

Name	Formula	ρ_p , g/cc	Type	HUG	EEI	DSH	CS	EX	FSV
Aluminum, 1000	wt% Al-50.27(Fe-0.31)(Cu-0.07)(Mg-0.03)(Mn-0.03)(Si-0.01)(Ti-0.01)	2.7	Alloys	<input type="checkbox"/>					
Aluminum 5117	wt% Al-2x(0.5-1)(Cu-0.05)(Mg-0.1-0.3)(Mn-0.05-0.1)(Fe-0.05-0.1)	2.028	Alloys	<input type="checkbox"/>					
Aluminum nitride	AlN	3.21	Solid compounds and minerals	<input type="checkbox"/>					
Aluminum oxide, amorph.	Al ₂ O ₃	3.98	Solid compounds and minerals	<input type="checkbox"/>					
Aluminum-quartz nitride (50-50)	wt% SiO ₂ (50)AlN(50)	2.684	Minerals	<input type="checkbox"/>					
Aluminum-quartz nitride (60-40)	wt% SiO ₂ (60)AlN(40)	2.683	Minerals	<input type="checkbox"/>					
Aluminum-quartz nitride (70-30)	wt% SiO ₂ (70)AlN(30)	2.67	Minerals	<input type="checkbox"/>					
Aluminum	Al	2.712	Elements	<input type="checkbox"/>					
Aluminum, 1300		2.712	Alloys	<input type="checkbox"/>					
Aluminum, 2024	wt% Al-Cu-0.9-4.9(Mg) 2-4.8(Mn-0.3-4.9)	2.784	Alloys	<input type="checkbox"/>					

Definitions:
 ρ_p - initial density of substance
 HUG - shock compression data
 EEI - adiabatic expansion data
 DSH - double shock compression data
 CS - measurements of sound velocity behind shock front
 EX - isobaric expansion data ("exploding wires")
 FSV - free surface velocity profiles

Search capabilities should be improved, more search criteria should be added



Experimental Points: Tabular and Textual Representation

[Home page | References | New search]

Experimental data

Select substance: to get the desired substance

Aluminum, 1000, ρ_p 2.700 g/cc, wt% Al-50.27(Fe-0.31)(Cu-0.07)(Mg-0.03)(Mn-0.03)(Si-0.01)(Ti-0.01)

u	E , km/s	D , km/s	Remark	References
1.000	1.450	7.310	TD = 17 K	1. M. von Thiel (Ed.) 1977
	1.800	7.750	TD = 17 K	
	2.210	8.140	TD = 17 K	
	2.460	8.770	TD = 17 K	
	2.580	9.080	TD = 17 K	
	2.700	9.820	TD = 17 K	
	2.710	9.130	TD = 17 K	
	2.770	8.760	TD = 17 K	
1.041	2.230	8.240	TD = 347 K	
	2.500	8.500	TD = 347 K	
	2.790	8.830	TD = 347 K	

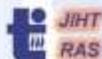
Aluminum oxide
 Double shot

u	E_1 , km/s	P_1 , GPa	dU_{12} , km/s
1.000	0.128	0.900	-0.712
	0.253	11.100	-0.707
	0.382	11.400	-0.223

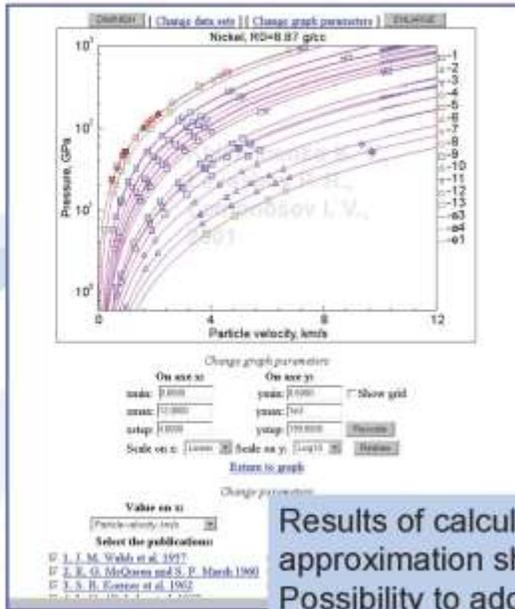
References:
 1. M. von Thiel (Ed.), Compression of Shock Wave Data, (Limestone) Lawrence Livermore Laboratory Report 808-08-08, 1971, 81-83

Summary:
 1.000 2.700 8.830 1 1
 1.041 2.790 8.830 1 1

References should be stored as a bibliographic records; Possibility to obtain references in different formats should be added



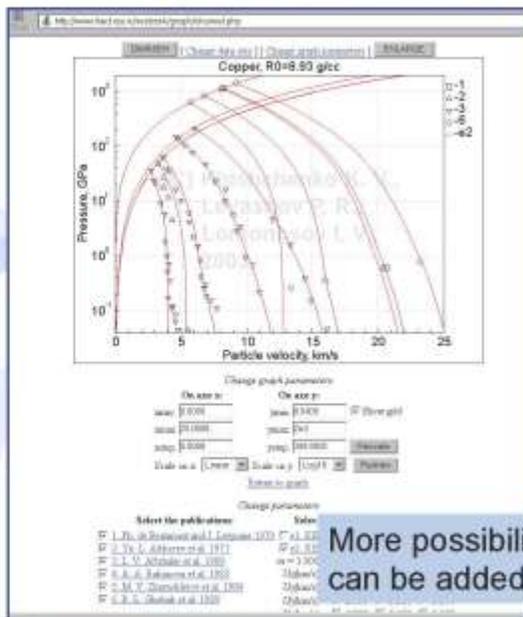
Shock Compression of Nickel



- 1-13 – experimental data on shock compression of nickel samples of different initial densities
- a3 – approximation of shock-wave data
- a4 – approximation of quantum-statistical calculations
- e1 – calculation on semi-empirical equation of state

Results of calculations by EOS or approximation should be available
 Possibility to add approximations by a user?

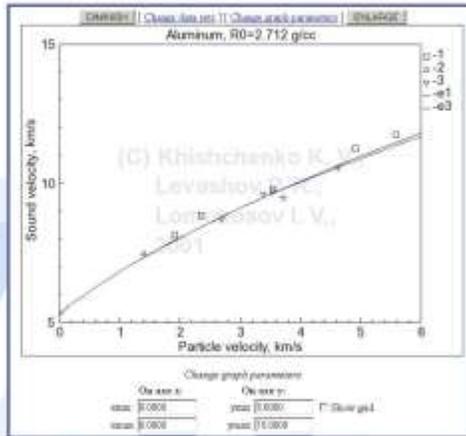
Isentropic Expansion of Copper



- 1, 2, 3, 6 – experimental data on isentropic expansion of copper samples with different initial densities
- e1 – calculation on semi-empirical equation of state

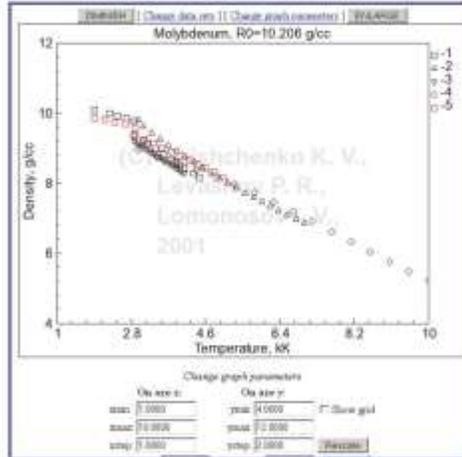
More possibilities to represent graphics can be added using client-side code

SOUND VELOCITY IN SHOCKED ALUMINUM



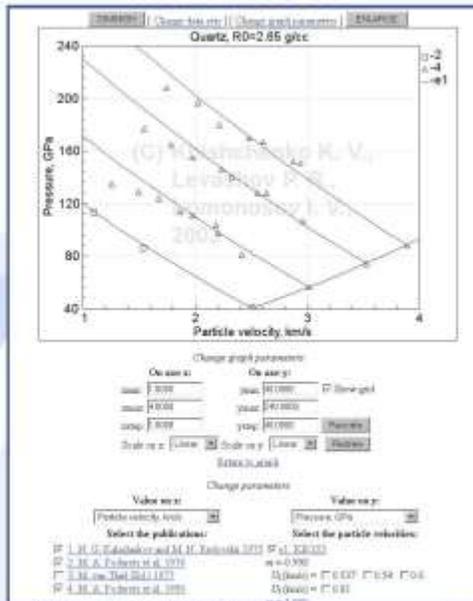
1-3 – experimental data
e1, e3 – equation of state calculations

ISOBARIC EXPANSION (μ s-electrical explosion) OF MOLYBDENUM



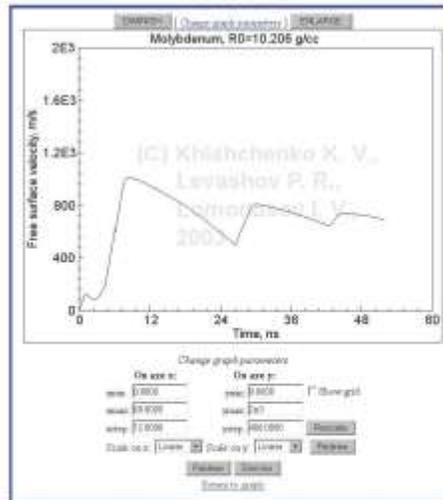
1-5 – experimental data

QUARTZ DOUBLE COMPRESSION



2, 4 – experimental data
e1 – equation of state calculation

FREE SURFACE VELOCITY PROFILE

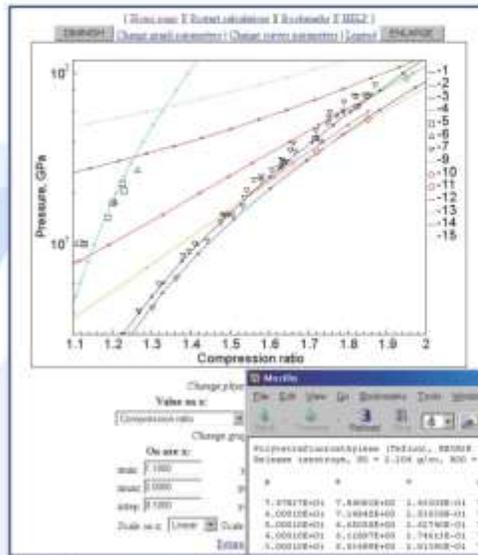


Free surface velocity profile
Sample: Mo, 0.416 mm thick
Striker: Al, 0.05 mm thick,
velocity 4100 km/c

TEFLON: EOS CALCULATIONS

Different curves calculated using semi-empirical EOS for teflon. Graphical and numerical representation of calculation results

Description of calculated curves and experimental points for teflon



1. Calculation, Shock Hugoniot, Polytropic equation (Teflon), EOSCE, $A_0 = 2.204$ g/cc, $A_1 = 2.204$ g/cc, $w = 1.000$, Output
2. Calculation, Helmholtz integrals, Polytropic equation (Teflon), EOSCE, $A_0 = 2.204$ g/cc, $A_1 = 2.204$ g/cc, $w = 1.000$, $C_0 = 3.964$ kcal/mole, Output
3. Calculation, Cold curve, Polytropic equation (Teflon), EOSCE, Output
4. Calculation, Double shock, Polytropic equation (Teflon), EOSCE, $A_0 = 2.204$ g/cc, $A_1 = 2.204$ g/cc, $w = 1.000$, $C_0 = 3.964$ kcal/mole, Output
5. Experiment, Shock Hugoniot, Polytropic equation (Teflon), M. van Thiel (2011) 1977, $A_0 = 2.204$ g/cc, $A_1 = 0.761$ g/cc, $w = 2.023$, Output
6. Experiment, Shock Hugoniot, Polytropic equation (Teflon), M. van Thiel (2011) 1977, $A_0 = 2.204$ g/cc, $A_1 = 0.761$ g/cc, $w = 2.024$, Output
7. Experiment, Shock Hugoniot, Polytropic equation (Teflon), G. F. Mack (2011) 2005, $A_0 = 2.204$ g/cc, $A_1 = 2.152$ g/cc, $w = 1.024$, Output
8. Experiment, Helmholtz integrals, Polytropic equation (Teflon), A. V. Stepanov et al. (2005), $A_0 = 2.204$ g/cc, $A_1 = 2.204$ g/cc, $w = 1.000$, $C_0 = 3.969$ kcal/mole, Output
9. Calculation, Shock Hugoniot, Polytropic equation (Teflon), EOSCE, $A_0 = 2.204$ g/cc, $A_1 = 0.761$ g/cc, $w = 2.024$, Output
10. Experiment, Double shock, Polytropic equation (Teflon), D. B. Zerk (2001) et al. (1970), $A_0 = 2.204$ g/cc, $A_1 = 2.197$ g/cc, $C_0 = 3.960$ kcal/mole, Output
11. Experiment, Double shock, Polytropic equation (Teflon), E. B. Zerk (2001) et al. (1970), $A_0 = 2.204$ g/cc, $A_1 = 2.197$ g/cc, $C_0 = 3.929$ kcal/mole, Output
12. Calculation, Double shock, Polytropic equation (Teflon), EOSCE, $A_0 = 2.204$ g/cc, $A_1 = 2.204$ g/cc, $w = 1.000$, $C_0 = 3.964$ kcal/mole, Output
13. Calculation, Isomerg, Polytropic equation (Teflon), EOSCE, $A_0 = 1.999$ kJ/g, Output
14. Calculation, Isomerg, Polytropic equation (Teflon), EOSCE, $A_0 = 23.000$ kJ/g, Output
15. Calculation, Isomerg, Polytropic equation (Teflon), EOSCE, $A_0 = 30.000$ kJ/g, Output

Modeling of Typical Shock-Wave Experiments

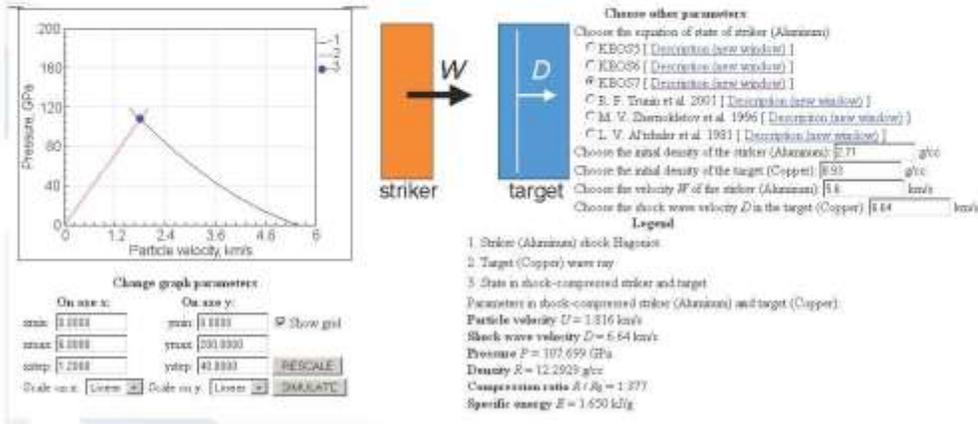
- «Collision» and «Impedance matching» methods
- 3 types of experimental set-ups for each methods
- Riemann problem is solved with given accuracy using shock Hugoniot approximations and EOSs
- User can choose materials of all substances participating in the experiment, their initial density and EOSs
- Modeling results can be presented in graphical (in pressure-particle velocity diagram) and textual form
- The interface allows one to estimate the influence of EOS or shock Hugoniot approximation on the interpretation of experimental data

«COLLISION» METHOD

Striker: aluminum, KEOS7 EOS, $W = 5.6$ km/s
 Target: copper, $D = 6.64$ km/s

- A1. Given are W , D , and striker shock Hugoniot. Determine pressure P and particle velocity U in shock-compressed striker and target, as well as density ρ and specific internal energy E of the target.
 A2. Given are striker velocity W and shock Hugonots or EOSs of striker and target. Determine the shock wave velocity D and parameters P , U , ρ , and E in the target.
 A3. Given are shock wave velocity in the target D and shock Hugonots or EOSs of striker and target. Determine the target velocity W and parameters P , U , ρ , and E behind shock wave front in the target.

Experiment: Altshuler L.V., Korner S.B., Bakanova A.A., Trunin R.F. // JETP. 1960. V.38. №3. P.790.

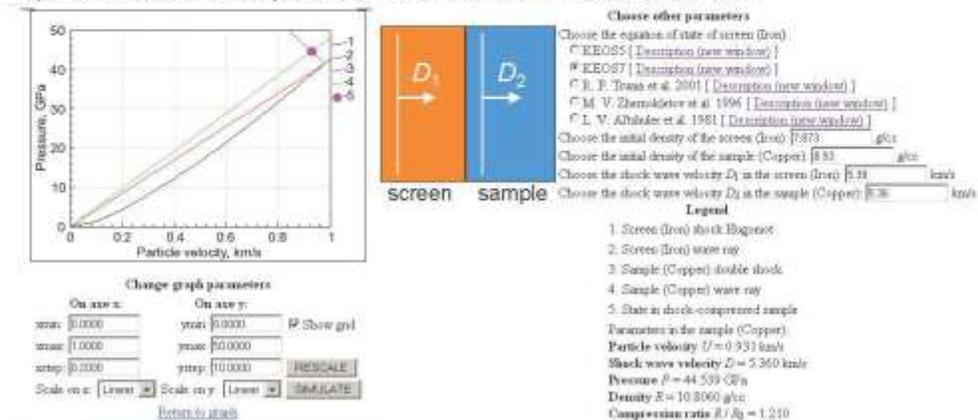


«IMPEDANCE MATCHING» METHOD

Screen: iron, KEOS7 EOS, $D_1 = 5.38$ km/s
 Sample: copper, $D_2 = 5.36$ km/s

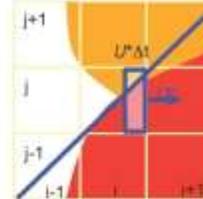
- B1. Given are shock wave velocities in the screen D_1 and in the sample D_2 , as well as shock Hugoniot or EOS of the screen. Determine parameters P , U , ρ , and E in the shock-compressed sample.
 B2. Given are shock wave velocity in the screen D_1 , and shock Hugoniot or EOSs of screen and sample. Determine shock wave velocity in the sample D_2 and parameters P , U , ρ , and E behind the shock front.
 B3. Given is the shock wave velocity in the sample D_2 . Determine the shock wave velocity in the screen D_1 and parameters P , U , ρ , and E of the sample behind the shock front.

Experiment: Altshuler L.V., Krupnikov K.K., Brazhnik M.I. // JETP. 1960. V.34. №4. P.886.



HYDROCODE

1. Multi-material high-order Godunov method in Eulerian form (Miller & Puckett, J. Comp. Phys., 1996)
2. Interface reconstruction algorithm (Youngs)
3. Equations of state (Khishchenko)



$$\frac{\partial f^\alpha}{\partial t} + \nabla \cdot (f^\alpha \mathbf{u}) = \frac{f^\alpha K_S}{K_S^\alpha} \nabla \cdot \mathbf{u}$$

$$\frac{\partial (f^\alpha \rho^\alpha)}{\partial t} + \nabla \cdot (f^\alpha \rho^\alpha \mathbf{u}) = 0$$

$$\frac{\partial (\bar{\rho} \mathbf{u})}{\partial t} + \nabla \cdot (\bar{\rho} \mathbf{u} \otimes \mathbf{u}) + \nabla \bar{P} = 0$$

$$\frac{\partial}{\partial t} \left[f^\alpha \rho^\alpha \left(E^\alpha + \frac{|\mathbf{u}|^2}{2} \right) \right] + \nabla \cdot \left[f^\alpha \rho^\alpha \left(E^\alpha + \frac{|\mathbf{u}|^2}{2} \right) \mathbf{u} + \bar{P} \mathbf{u} \right] = 0$$

$$\sum_\alpha f^\alpha = 1$$

$$\bar{\rho} = \sum_\alpha f^\alpha \rho^\alpha$$

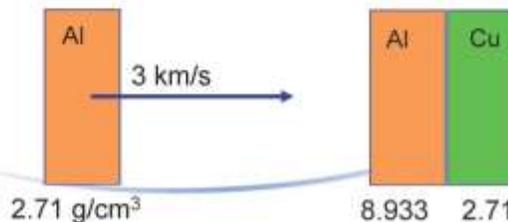
$$1/\bar{K}_S = \sum_\alpha f^\alpha / K_S^\alpha$$

$$\bar{P} = \sum_\alpha \frac{f^\alpha P^\alpha}{K_S^\alpha} / \sum_\alpha \frac{f^\alpha}{K_S^\alpha}$$



Principles and Technical Aspects of the ISWdb, Oct 31 2011

SCELETON OF INTERFACE: STEP 1



SCELETON OF INTERFACE: STEP 2

Choose parameters for the objects

Object 1:

Choose substance:

Aluminum

Insert the position of object 1 in mm (from 0 to 20 mm):

0

Insert the thickness of object 1 in mm (from 0.1 to 5 mm):

2

Insert the velocity of object 1 in km/s (from -20 to 20 km/s):

3

Insert the minimal spall strength of object 1 in GPa (from -50 to -0.1 GPa):

-2

Object 2:

Choose substance:

Aluminum

Insert the position of object 2 in mm (from 0 to 20 mm):



SCELETON OF INTERFACE: STEP 3

Choose the equations of state:

Aluminum

Density: 2.71 g/cc

Pressure: 10^{-4} GPa

Choose EOS:

Choose the equation of state for Aluminum: KEOS3

Aluminum

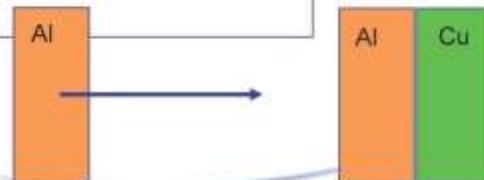
Density: 2.71 g/cc

Pressure: 10^{-4} GPa

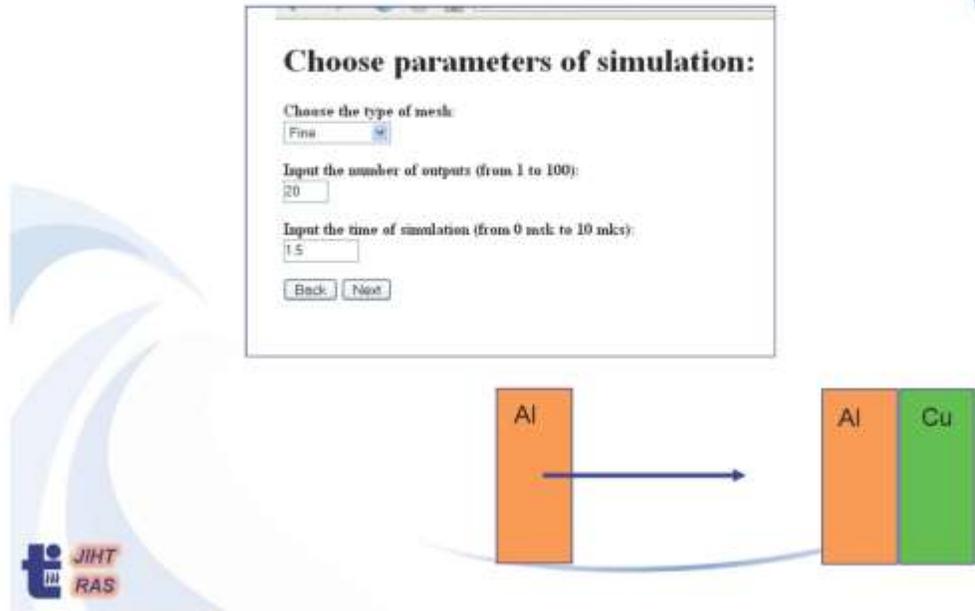
Choose EOS:

Choose the equation of state for Aluminum: KEOS3

Copper



SCELETON OF INTERFACE: STEP 4



Choose parameters of simulation:

Choose the type of mesh:
Fine

Input the number of outputs (from 1 to 100):
20

Input the time of simulation (from 0 mcs to 10 mcs):
1.5

Back Next

Al → Al Cu

The screenshot shows a window titled "Choose parameters of simulation:" with three input fields: a dropdown menu for "Choose the type of mesh" set to "Fine", a text box for "Input the number of outputs (from 1 to 100)" containing "20", and a text box for "Input the time of simulation (from 0 mcs to 10 mcs)" containing "1.5". Below the fields are "Back" and "Next" buttons. To the right, a diagram shows an orange bar labeled "Al" with an arrow pointing to a combined orange and green bar labeled "Al" and "Cu".

SCELETON OF INTERFACE: STEP 5



Configuration file has been created

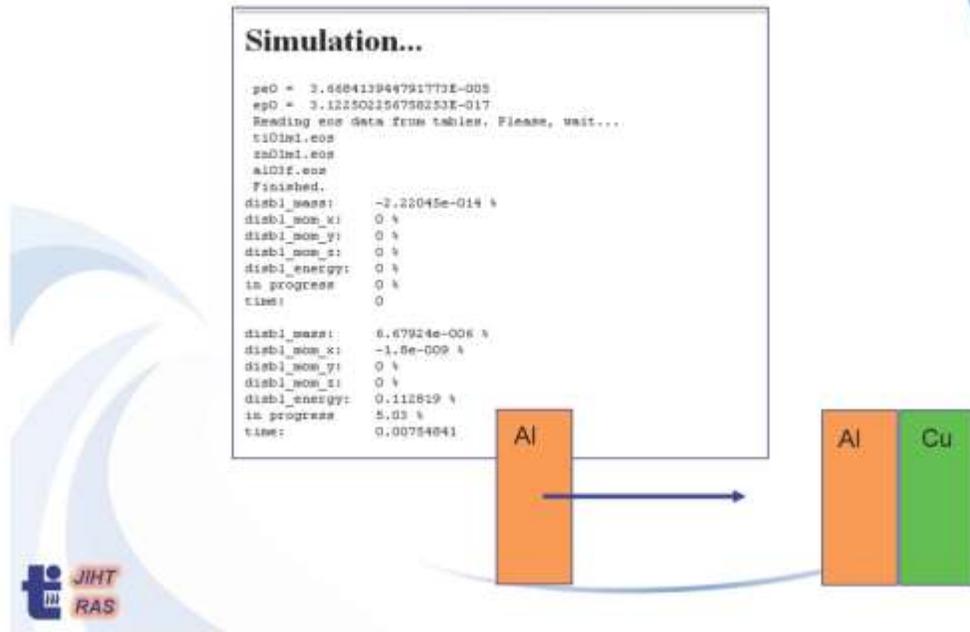
```
pe0 = 3.600413044791773E-005  
ep0 = 3.122502226759253E-017  
Reading eos data from tables. Please, wait...  
t101ml.eos  
m101ml.eos  
s101f.eos  
Finished.  
Memory allocated: 2489 KB
```

Start simulation

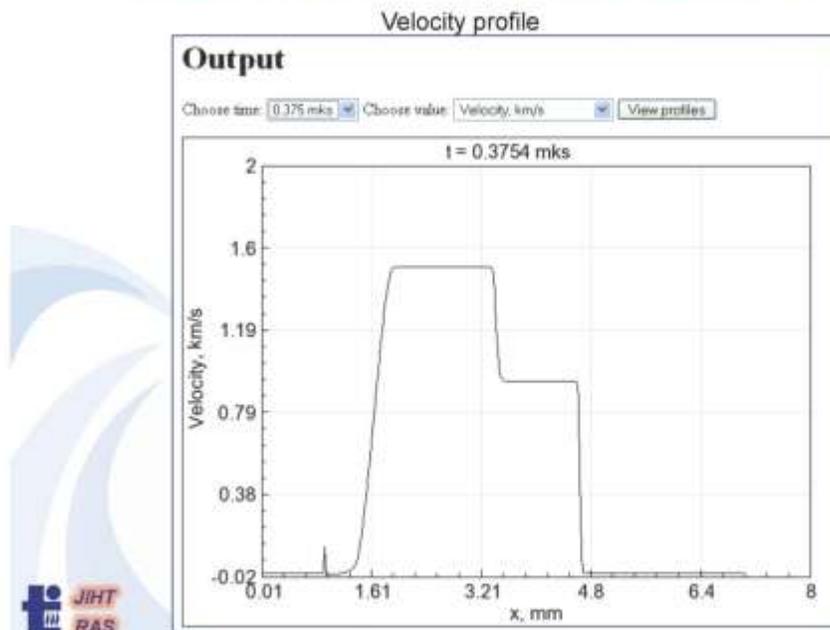
Al → Al Cu

The screenshot shows a window titled "Configuration file has been created" with a text area containing simulation parameters and a "Start simulation" button. To the right, a diagram shows an orange bar labeled "Al" with an arrow pointing to a combined orange and green bar labeled "Al" and "Cu".

SCELETON OF INTERFACE: STEP 6

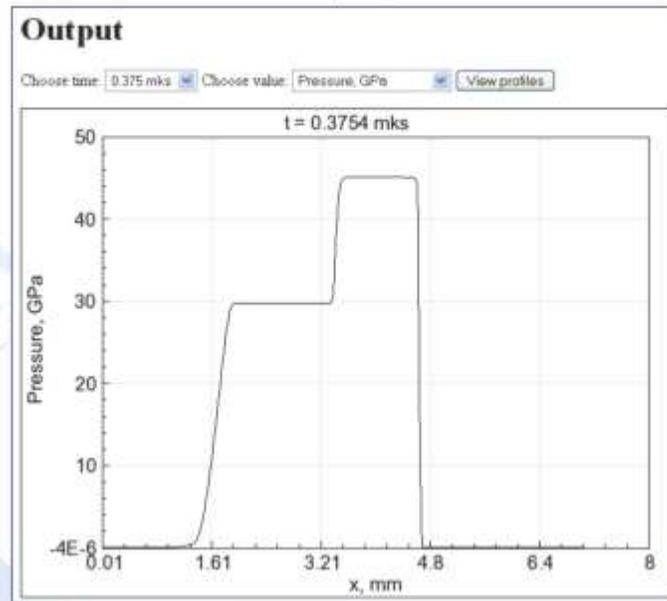


SCELETON OF INTERFACE: STEP 7



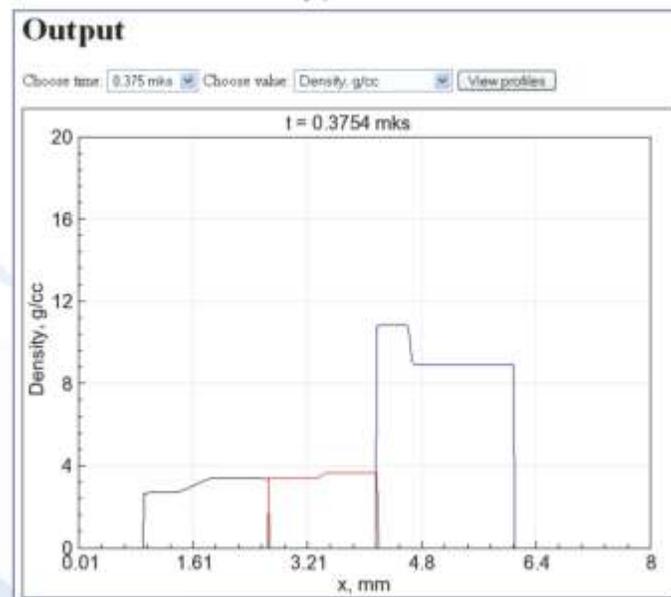
SCELETON OF INTERFACE: STEP 7

Pressure profile



SCELETON OF INTERFACE: STEP 7

Density profile



ISWdb: First Steps

- Decide which types of experimental data will be available in the database
- Define the textual format for each data type (XML?)
- Create the convertors from these formats to SQL and store data into the database
- Create a simple web-interface for viewing and editing data

Discuss and implement other modules (Web-interface)



Sandia National Laboratories

International Shock Wave Database Workshop
Darmstadt, Germany,
November 1, 2011

International Shock Wave Database: Sandia Perspective

Seth Root

sroot@sandia.gov

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.




Sandia Experimental Facilities





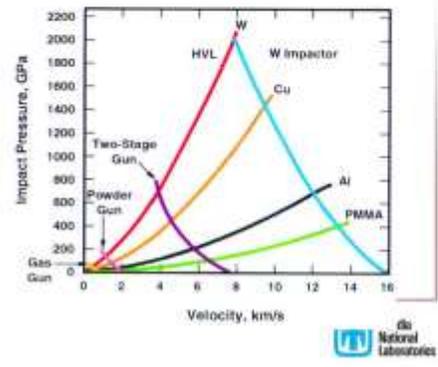


- The goal of these facilities is to provide dynamic compression data used for Equation of State and Constitutive Model development.



STAR Facility

- Shock Thermodynamic Appled Research
- Dynamic loading experimental test facility
- Operational since the mid-1960s
- Several launchers capable of velocities from 50 m/s to ~8 km/s
- Wide range of attainable pressures using variable impactors



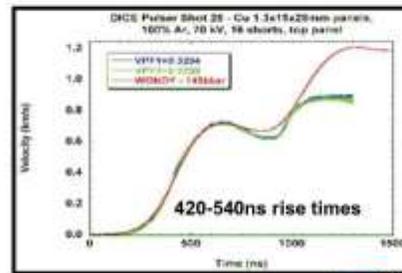
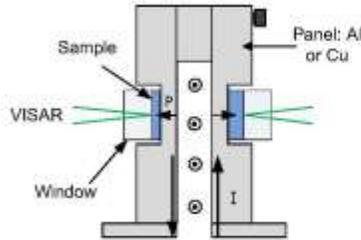
STAR Launchers

Launcher	Diameter (mm)	Velocity (km/s)	Uses
1-stage, gas	100	0.1 – 1	Shock
1-stage, powder	89	0.4 – 2.2	Shock
Oblique Impact	100	0.05 – 0.35	Pressure/Shear
2-stage	20, 30, 67	0.8 – 7.5	Shock
Terminal Ballistic	6 – 30	0.8 – 7.5	Penetration Studies



DICE Facility Capabilities

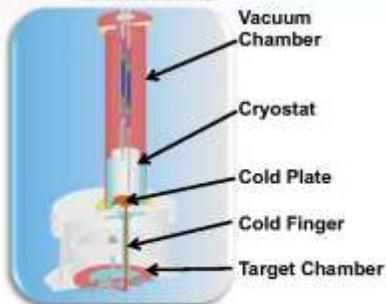
VELOCE Shock-less Compression System



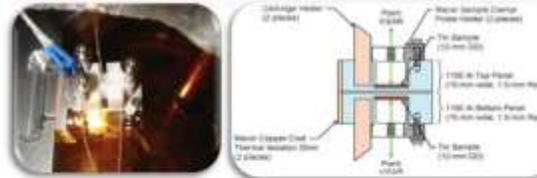
- 2.6 MA of current – 4 to 14 GPa
- Point VISAR and Line VISAR
- EOS, phase transitions, strength

VELOCE Temperature Control

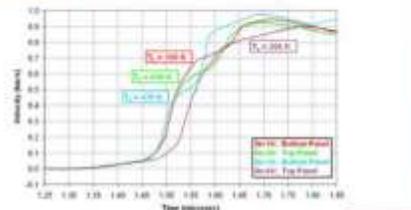
Pre-Cooling



Pre-Heating

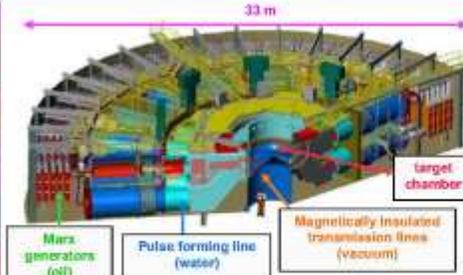
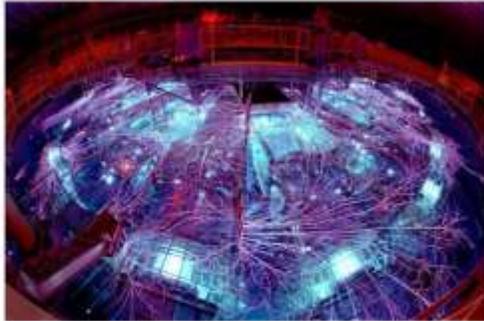


- Pre-cooling using LN₂ (in development)
- Pre-heating: 25°C to 200°C
- Examine temperature effects and phase boundaries



Wise, et al., "Measurement of the temperature dependence of the β - γ transition pressure in tin using dynamic isentropic compression," Shock Compression of Condensed Matter 2008, Chicago.

Sandia Z - Machine



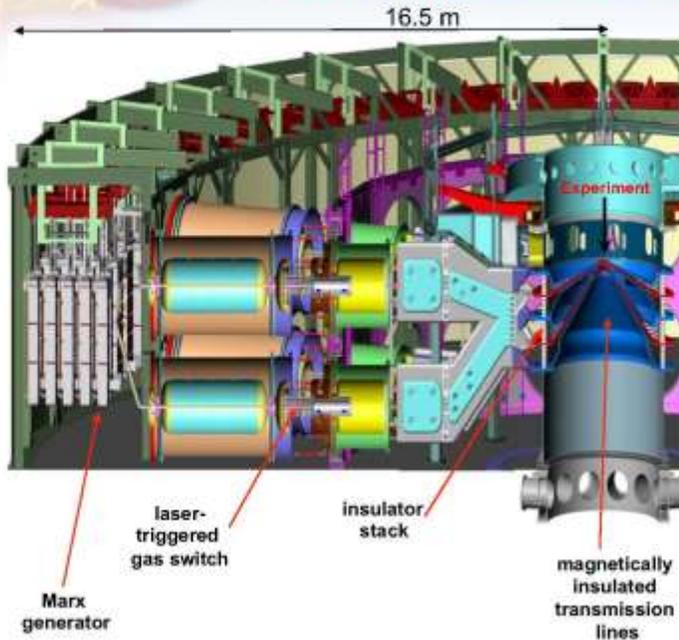
• 26 MA, 100-700 ns

- 2.65×10^6 L of oil
- 1.14×10^6 L of water
- 33 m in diameter
- 5 m in height



Sandia National Laboratories

The Sandia Z Machine



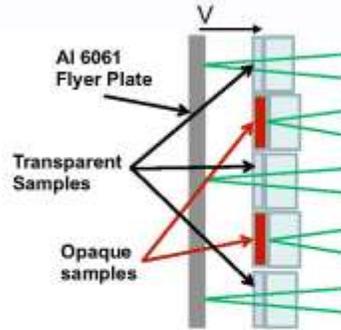
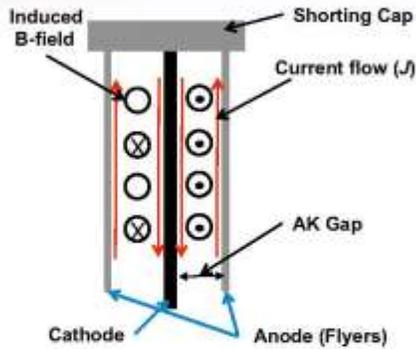
22 MJ stored energy
~26 MA peak current
~100-700 ns rise time



Experimental Target

Sandia National Laboratories

Shock Compression

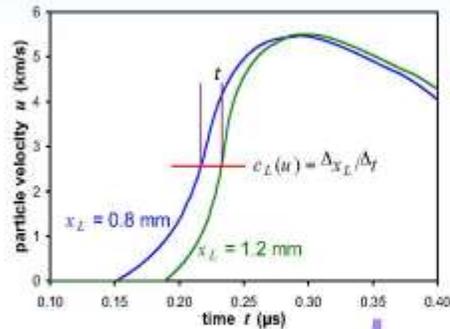
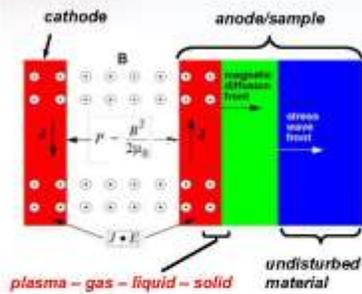


- Current pulse loops through shorting cap inducing a B - field.
- Resulting $J \times B$ force accelerates anodes (flyers) outward up to 40 km/s
- Asymmetric AK Gaps result in two different flyer velocities (two Hugoniot points per experiment)

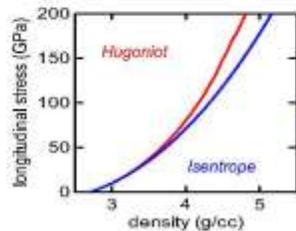
- Multiple samples per experiment
- Flyer velocities up to 40 km/s
- VISAR used to measure flyer velocity
- Hugoniot data to pressures > 10 Mbar



Shock-less Compression



- EOS Data
- Phase Transitions
- Strength
- up to 4 Mbar

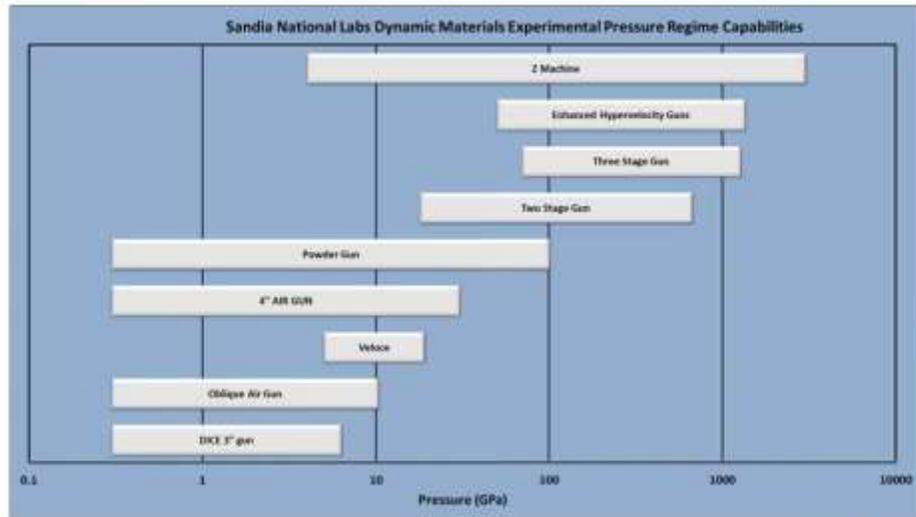


$$d\sigma_x = \rho_0 c_L du$$

$$\frac{d\rho}{\rho^2} = \frac{du}{\rho_0 c_L}$$



Accessible Regimes



Requirements and Features for the International Shock Wave Database



Type of Data Collected

- Shock Hugoniot data
- Double shock and shock – release data
- Explosives: unreacted Hugoniot and Shock – Detonation Transition data (?)
- Isentrope data from shock-less compression
- Wave profile measurements from shock and shock-less compression data
- Sound speed data

Other Useful Data

- Thermodynamic data: specific heat, thermal expansion, etc
- Static compression isothermal data
- Phase diagrams
- Strength information (elastic-perfectly plastic, Steinberg-Guinan parameters, etc)



Contributed Data Requirements

- $U_S - U_P$ or $U_S - U_{FS}$, Flyer Velocity, ρ_0
 - Measured values, not derived quantities
- Experimental Method:
 - Plate Impact, HE Driven, Direct Laser Drive
 - Pins, imbedded gauges, VISAR, PDV, etc
- Measurement Uncertainty / Error
- Impedance Matching Standard
- Data published in peer-reviewed Journal AND/OR approved by ISWDb review committee
 - Free surface data requires an assumption about the release isentrope – typically assume some release follows a Mie-Gruneisen relation, which requires Γ_0



Impedance Matching Standards

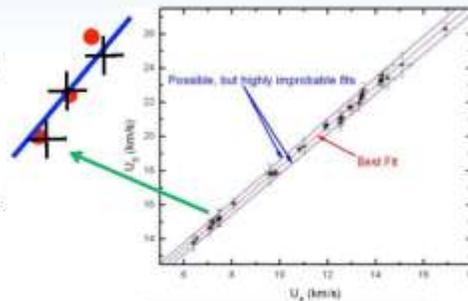
- Ideally, all shock data would be acquired using symmetric impact or a set of well-characterized impedance standards.
- The database should maintain up-to-date and thoroughly analyzed (and reanalyzed) data for a series of shock impedance standards
- Aluminum 1100, 2024, and 6061
- Copper
- Tantalum
- Window materials: Quartz, Sapphire, and LiF
- Data includes: **weighted, Monte Carlo – optimized fit parameters, parameter uncertainty, and covariance matrix for the parameters**
- **Database to be the authority on these standards, maintaining the latest data and most up-to-date characterization**



Monte Carlo (MC) Impedance Matching

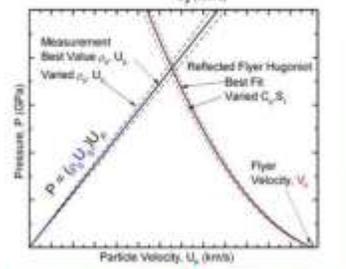
Aluminum

- Uncertainty in experimental data (Knudson *et al.*, JAP 2003)
- Vary each U_S - U_P point by an uncorrelated random number with $\sigma =$ expt uncertainty
- Solve for linear fit parameters and generate a distribution of fits
- Determine mean, σ , and correlation matrix of the fit parameters



Target Material

- Vary measured parameters (V_F , U_S , ρ_0) with uncorrelated random numbers, $\sigma =$ expt uncertainty
- Vary AI fit parameters using correlated random numbers
- Calculate U_p , P , and ρ
- Determine mean and σ



Monte Carlo technique accounts for experimental uncertainty and propagates error in the AI standard into the resulting target data.



Database Example

Aluminum Alloy

- 6061 – T6
- 1100
- 2024
- 7075
- Shock Data
- Release Isentrope
- Compression Isentropes
- Isotherms
- Strength Parameters

Properties

$$\rho_0 = 2.712 \text{ g/cm}^3$$

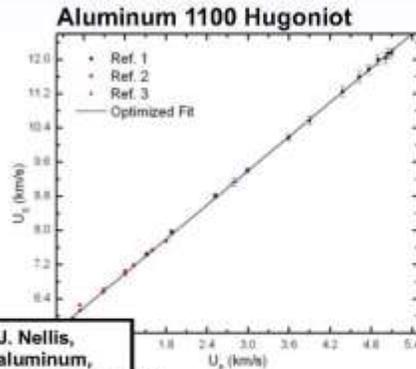
$$C_L = 6.36 \text{ km/s}$$

$$C_S = 3.16 \text{ km/s}$$

$$\Gamma_0 = 2.14$$

$$C_p(T) = m_1 + m_2 f(t) + m_3 f(t^2) + \dots$$

[1] A. C. Mitchell and W. J. Nellis, "Shock compression of aluminum, copper, and tantalum." J. Appl. Phys. 52, 3363, (1981).



$$\text{Fit: } U_s = 5.396(-0.021) + 1.335(+0.012)U_p$$

Covariance Matrix =

1.499e-4	-2.253e-4
-2.253e-4	4.597e-4



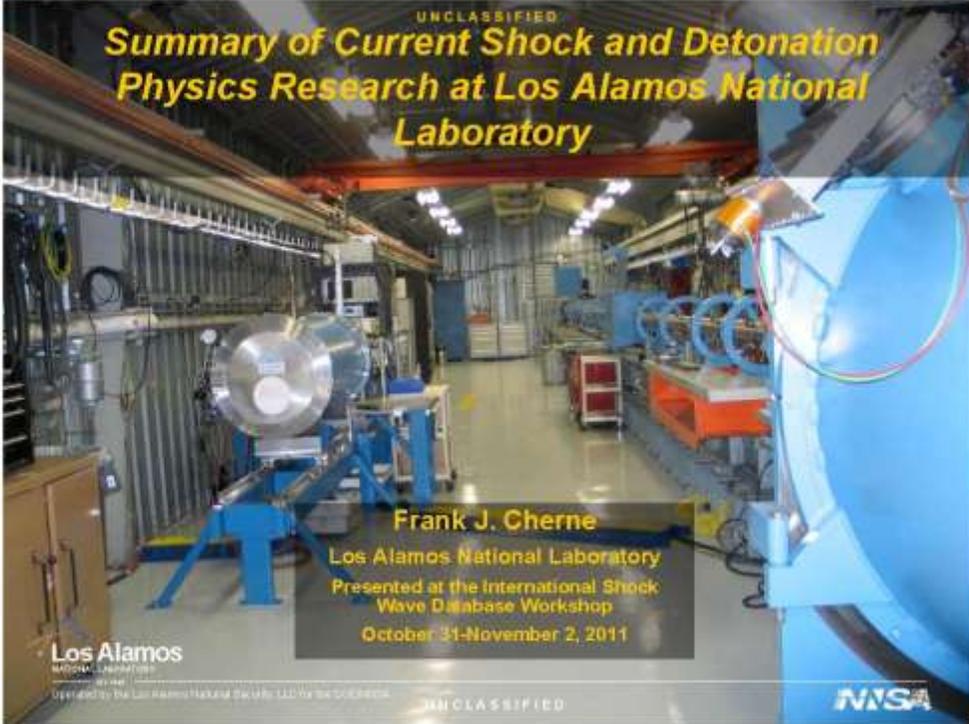
Challenges for the ISWDb

- Find and archiving original data – many older papers show plots, but no data tables
- Finding uncertainties for the measured data
- Mixed impedance matching standards
 - Data on Al Hugoniot was generated using Ta impactors, but some Ta data was collected with Al impactors
- All contributed data should be from peer-reviewed journals AND/OR reviewed by ISWDb committee. New data should be compared to old to verify consistency.
 - Deuterium Hugoniot: NOVA D_2 vs. Omega D_2 vs. Z D_2
- Encourage usage of the database and contributions to the database – Advertising: SCCM 2013 (US), SWCM 2012 (Russia), Others?
- Ensuring time and money for continual updates



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Summary of Current Shock and Detonation Physics Research at Los Alamos National Laboratory



Frank J. Cherne
Los Alamos National Laboratory
Presented at the International Shock Wave Database Workshop
October 31-November 2, 2011

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The people of the shock and detonation physics group



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WX-9: Shock and detonation physics group at LANL

- The group is a descendent of the legendary group that produced the data found in *LASL Shock Hugoniot Data* edited by S. Marsh
- Shock wave and isentropic loading techniques available:
 - Gas guns producing projectile velocities ranging from 0.15-8 km/s
 - Enclosed vessel for HE firing
 - Laser shock drivers
 - Sandia's Z machine
- Diagnostics available:
 - Photon Doppler Velocimetry
 - VISAR/Line VISAR
 - Magnetic Gauge
 - X-ray diffraction
 - Prad
 - Argonne Laboratory's APS synchrotron radiation source
 - Framing cameras and streak cameras

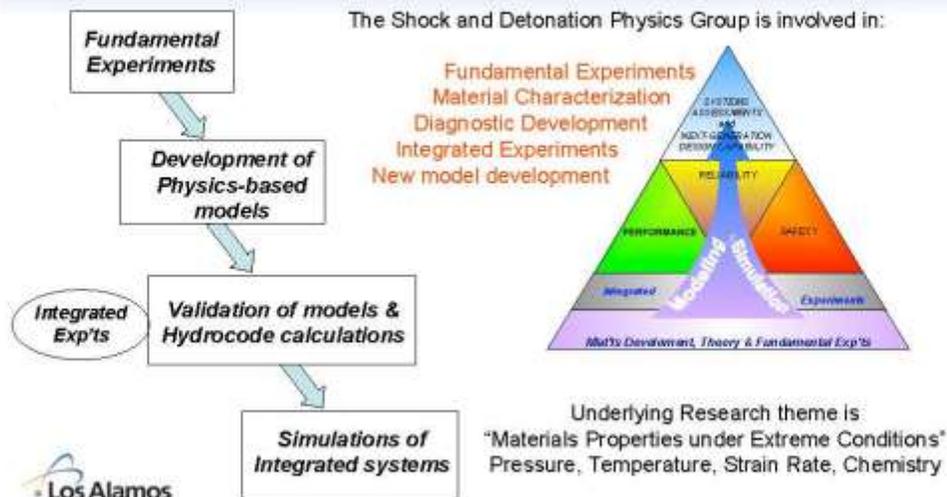


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Experimental activities in Shock and Detonation Physics at Los Alamos enable realistic simulations of our stockpile.



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Outline of the remainder of my talk

- A brief overview of some of the facilities that we use to produce shock wave data
- Several examples of shock wave data obtained
 - Metals
 - Polymers
 - High explosives
- Thoughts on the International Shockwave Database



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TA-39-56 – Single stage light gas gun

- Helium is quasi-statically pumped into the breech to accelerate projectiles to velocities of 0.1 – 0.8 km/s
- Unique capabilities
 - Open-air gun – fires into the canyon
 - No catch tank = high shot rate (> 50 shots per year)
 - New diagnostics and techniques can be fielded with little effort
 - Pre-heat, pre-cool, framing cameras, x-ray radiography
 - Materials such as lead and depleted uranium can be shot at this site



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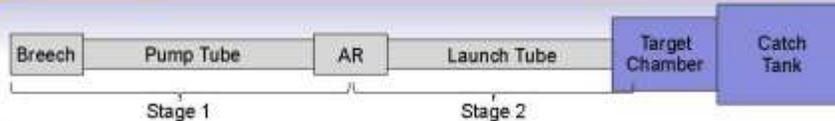


TA-39-69 – Single stage powder gun

- Up to 300g of rifle powder is used to accelerate projectiles to velocities of 0.25 – 2.0 km/s
- Unique Capabilities
 - Velocity range is well suited for studying phase transformations in wide variety of materials
 - Narrow target chamber has allowed the fielding of many types of diagnostics while providing protection of equipment
 - Dynamic x-ray (Bragg) diffraction
 - Infrared imaging using IR framing camera



TA-39-69 – High Performance two-stage light gas gun

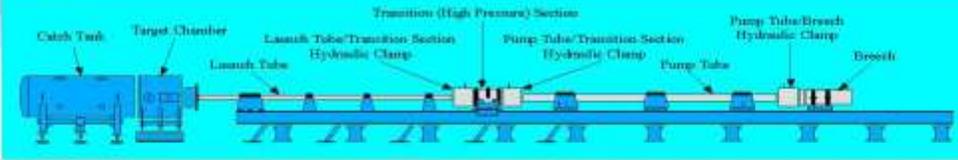


- Stage 1 is filled with 100 psi of gas (He or H₂)
- Up to 8 lbs. of military grade propellant are used to drive an 89mm piston in Stage 1 to dynamically compress the gas by 1000x
- This gas launches a 28mm projectile to velocities of 2 – 6+ km/s
- Higher velocities (up to 8 km/s) can be reached with a smaller diameter launch tube resulting in stresses in excess of 5 Mbar in metals.



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Gas-Gun Experiments Probe the Shock Behavior of Polymers and Explosives

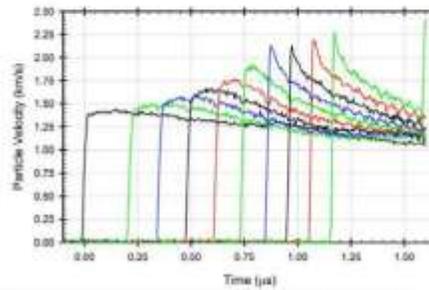
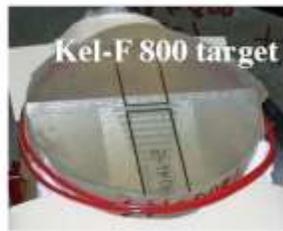


Large bore guns designed for high explosive experiments; also being applied to polymers & foams

Plate impact experiments – projectile velocities ~ 0.25 – 3.4 km/s
 Embedded (*in situ*) electromagnetic gauges give wave profiles



$$Voltage = L \cdot u_p \cdot B$$



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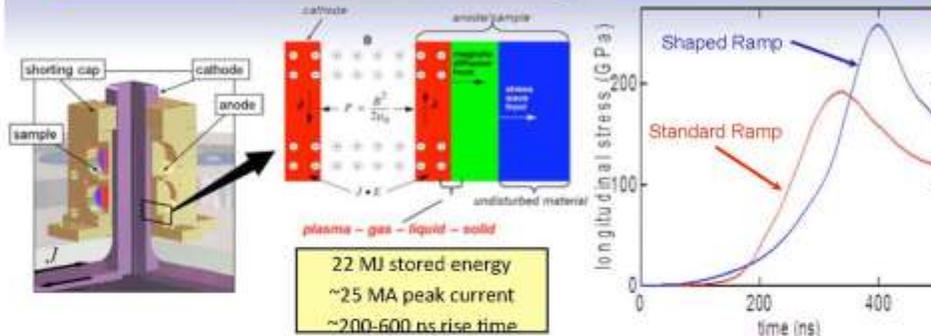
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Isentropic compression data can provide additional information about the kinetics of phase transformations



- Magnetic field between anode/cathode induces pressure on the sample
- Pressure pulse temporally follows current
 - This can be tailored by dumping capacitors sequentially
- Materials closely follow isentrope when ramp loaded.
- Isentrope will follow Hugoniot very closely for several hundred kbar.
- Same phase boundaries are accessible through shock and isentropic loading
- Phase transition cannot be "overdriven"
- Lower strain-rates allow investigation of strain-rate effects on phase transitions

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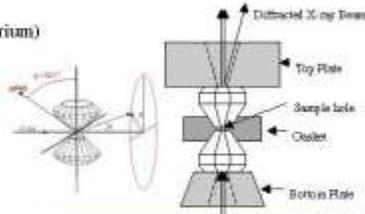
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Diamond Anvil Cell (DAC) Capabilities

- Used to obtain static equation of state info to very high stresses (> 1 Mbar)
- Cells can accommodate various experimental techniques – from x-ray diffraction to inelastic scattering to optical spectroscopies.
- Complement dynamic data
 - Lattice info (not bulk)
 - Isothermal data
 - Low to High Temp. (5000 K)
 - Low & High Pressure (4 Mbar)
 - EOS (pressure, volume, temp.)
 - Phase Diagram (equilibrium)
 - Lattice constants
 - Crystal structures
 - Phase boundaries
 - Volume changes
 - Strength Info.



Velocimetry is used in shock compression experiments to detect phase transitions in real time

Shock Compression Experiment



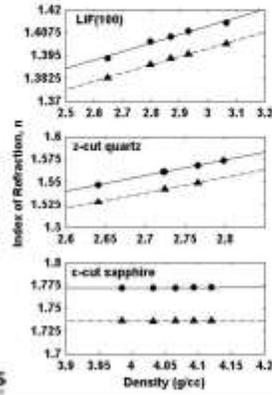
Application of PDV: velocities & window corrections

Impact jump to steady state

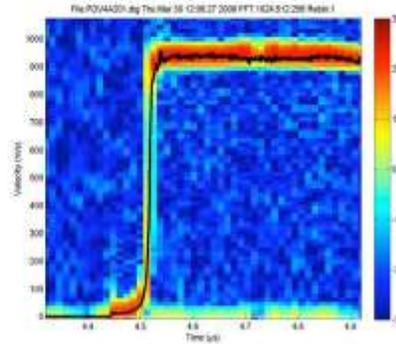
Velocity change as shock wave reflects from the free surface

PDV data more complex – Dan Dolan’s analysis explains features

Data useful for calculating window corrections, U_w , density, etc.



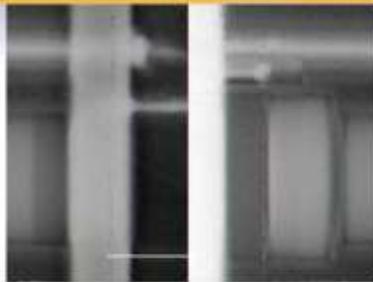
Jensen et al. JAP, 2007, 101, 013523.



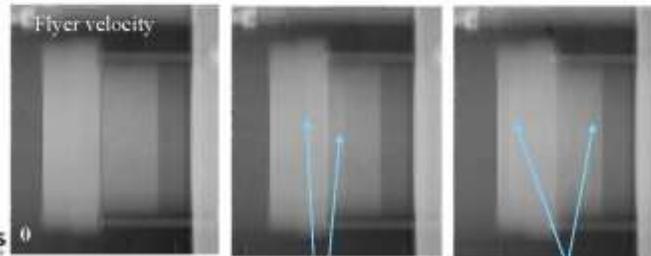
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Radiography Results – Aluminum Symmetric Impact



Rigg, Schwartz, Merrill, Morris et al. (2006)



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Density Calculations from Jump Conditions and radiographs agree well.

Impact Velocity

$$u_0 = 1.452 \pm 0.012 \text{ mm/ms}$$

Particle Velocity: $\frac{1}{2} u_0$

$$u_p = 0.726 \pm 0.006 \text{ mm/ms}$$

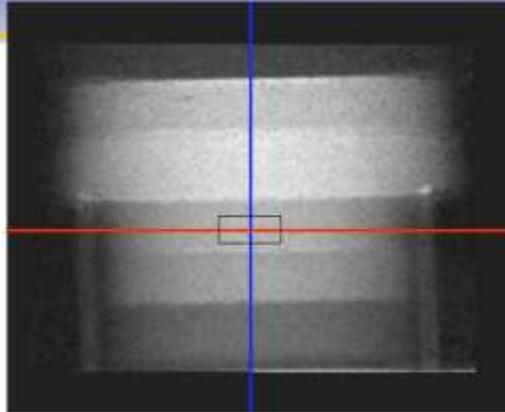
$P(u_p)$ for 6061-T6 Al

$$P = 1.184 + 140.2u_p + 37.38u_p^2$$

$$P = 12.27 \pm 0.09 \text{ GPa}$$

Initial density from immersion

$$r_0 = 2.710 \pm 0.003 \text{ g/cm}^3$$



Calculate density from Jump Conditions

Rigg, Schwartz, Merrill, Morris et al. (2006)

$$\rho = \frac{\rho_0 P}{P - \rho_0 u_p^2} \Rightarrow \rho = 3.067 \pm 0.009 \text{ g/cm}^3 \text{ (0.3\%)}$$

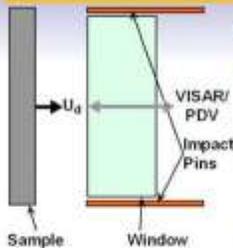


Density (radiography): $r = 3.07 \pm 0.03 \text{ g/cm}^3 \text{ (1.1\%)}$

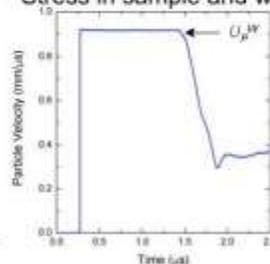
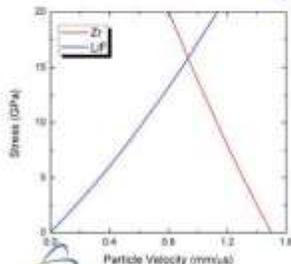
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Front surface impact (FSI) experiments eliminate wave interactions due to multi-wave structure



- Sample is impacted on window directly.
- Measurement of projectile velocity, U_d , and particle velocity, U_p^W , needed to determine Hugoniot point:
 - Projectile velocity measured using shoring pins or PDV to 0.1%.
 - Particle velocity measured at impact using VISAR and PDV to ~0.5 - 1%.



- Stress in sample and window defined by window Hugoniot

- Shock Velocity determined from R-H Jump Conditions:

$$U_s^S = \frac{P - P_1}{\rho_1(U_d - U_p^W - U_{p1})}$$

- Must know initial conditions!

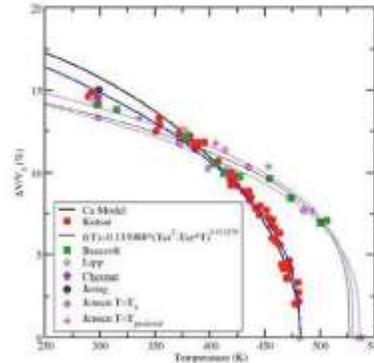


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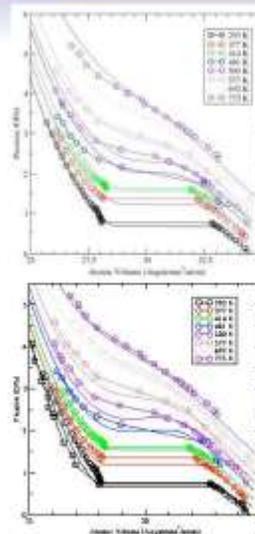
The wide assortment of data out there provides a unique challenge to fitting equations of state

- There are many experimental methods and measurements that have been used to provide information leading to the development of the equation of state. The major ones include:
 - Shock loading
 - Diamond anvil cell
 - Thermal expansion analysis
 - Specific heat measurements
 - Sound speed measurements
- Some data may not agree with other measurements
- Although equation of state parameters may describe one thermodynamic property another property may be poorly described.



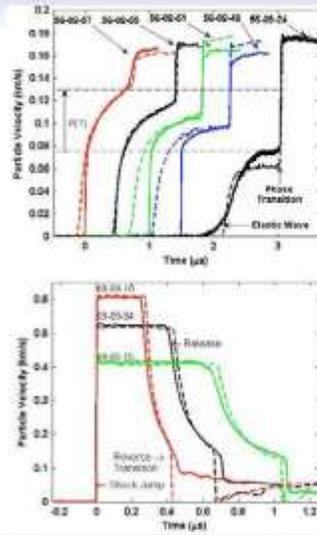
Comparing the model with isothermal compression data (DAC work performed by M. Lipp of LLNL)

- The model matches the isothermal data for the γ -phase
- The compressibility of α -phase shows that the model matches the room temperature isotherm almost exactly yet for higher temperatures the model is a little stiffer.
- The model predicts a lower phase transition pressure than the experiments.
- High pressure-high temperature is underway to probe the α - ϵ phase boundary.



The simulations of experimental data are in good agreement with the experimental data

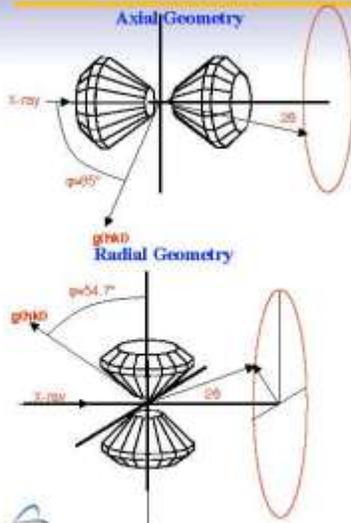
- Equation of state parameters were adjusted to better fit the following:
 - Compression data from Lipp
 - Volume collapse data
 - Adjusting the phase boundary slightly
- One dimensional hydrodynamic calculations were done in comparison with shock data
 - Transmission experiments show a good agreement for the phase transition for all experiments except for the room temperature experiment.
 - Front surface shots show good agreement
 - No strength or kinetics of phase transition included in the model.



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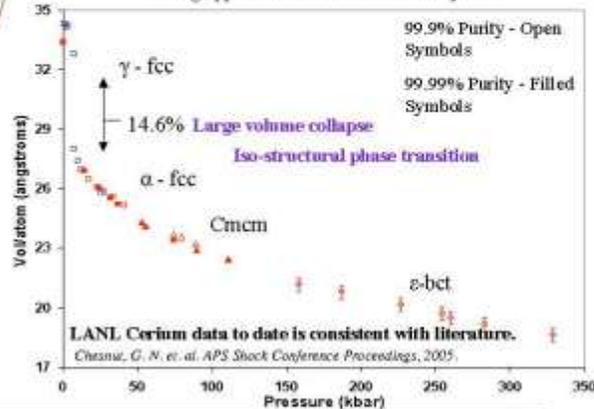
Dynamic Experiments are supported by x-ray diffraction at static high pressures in both axial and radial geometries.



Radial Diffraction can improve errors by a few percent - particularly for low symmetry structures.

Cerium is a good candidate material to test the validity of the radial method.

Being applied to new materials- Ti alloy etc.

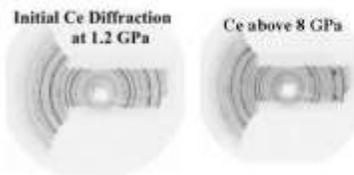
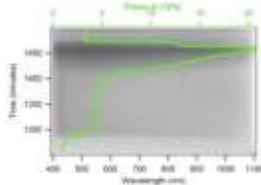


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X-ray Diffraction and Spectral Reflectometry Data Along the 500°C Isotherm in cerium (N. Velisavljevic)

- fcc indexed initially at 4 GPa
- At 8 GPa change in spectral reflectivity and significant grain growth observed

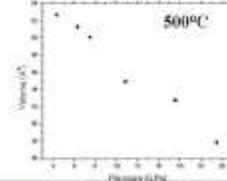


- Additional "single" crystal diffraction experiments performed, which show bct(ϵ) above 8 GPa and stable up to highest P reached (sample prepared by J. Cooley, LANL, and data collected in collaboration with O. Tschauer, UNLV)

X-ray single crystal diffraction

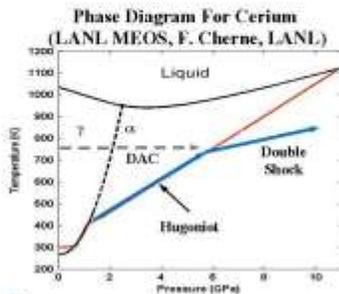


P-V data

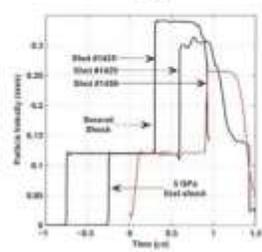
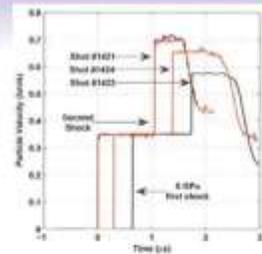
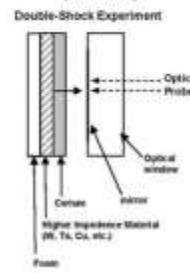


Dynamic data indicates that the ϵ -phase may be present in a similar P-T range

Multiple shock loading results in higher pressure states while minimizing the temperature
 Double-shock loading is used to obtain off-Hugoniot data to the "right" of the Hugoniot in the α - ϵ region of the phase diagram

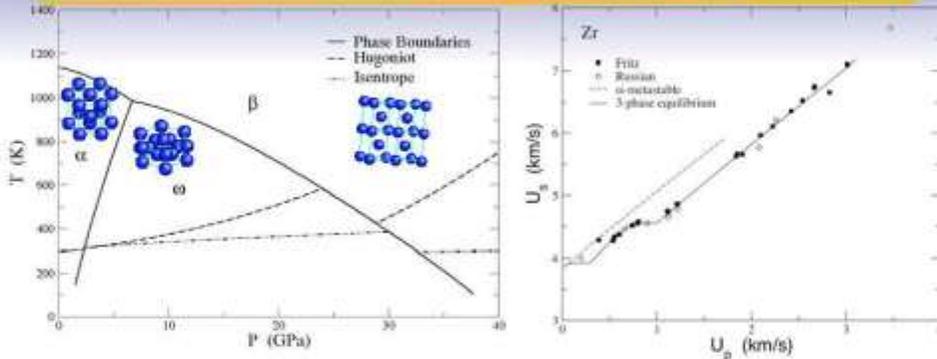


Double-Shock Experiment (B. Jensen)



B. J. Jensen and F. J. Cherne, LA-UR-10-06303

Zirconium is well suited for investigating solid-solid phase transitions under dynamic loading conditions



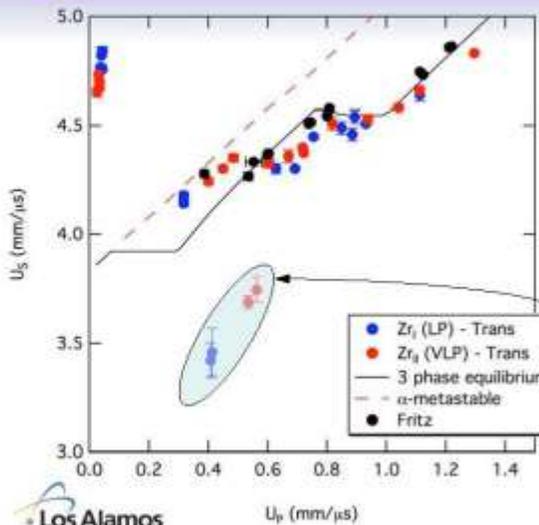
- Three solid phases exist in Zr in pressure regimes easily accessible through shock and isentropic loading.
- Kinks in legacy $U_s - U_p$ data indicate that transitions should be observable in shock compression experiments



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$U_s - U_p$ data obtained from shock experiments



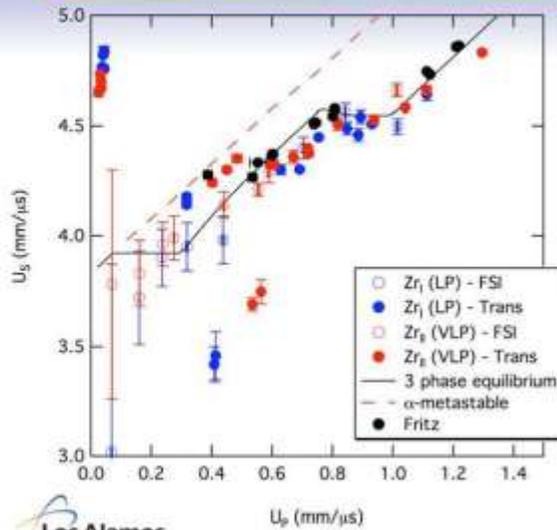
- The solid-solid phase transformations can be identified by kinks in $U_s - U_p$ data.
- Legacy data analyzed using single wave analysis resulting in artificially high U_s .
- α and ω phases may need to be shifted in Greeff EOS.
- Wave interactions not properly accounted for in extracting U_s from 3-wave profiles.



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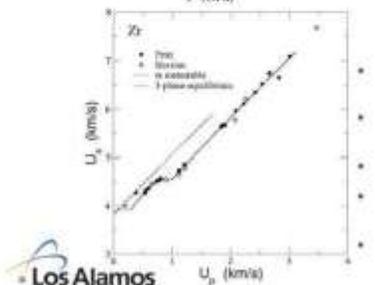
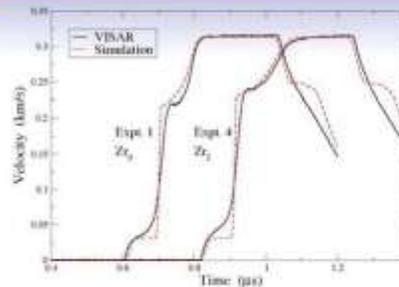
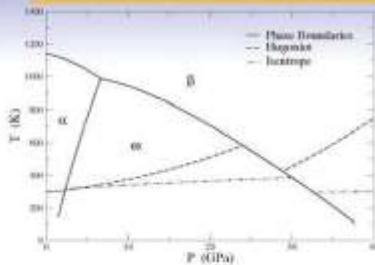


Calculated Hugoniot is in good agreement with data from front surface impact experiments



- Errors are large at low stresses due to uncertainties in initial state parameters.
- Results near the α - ω transition are more consistent with the calculated Hugoniot
 - Better measurement of equilibrium at transition??
- Transmission experiments seem to be better for determining the ω - β transition stress, but...

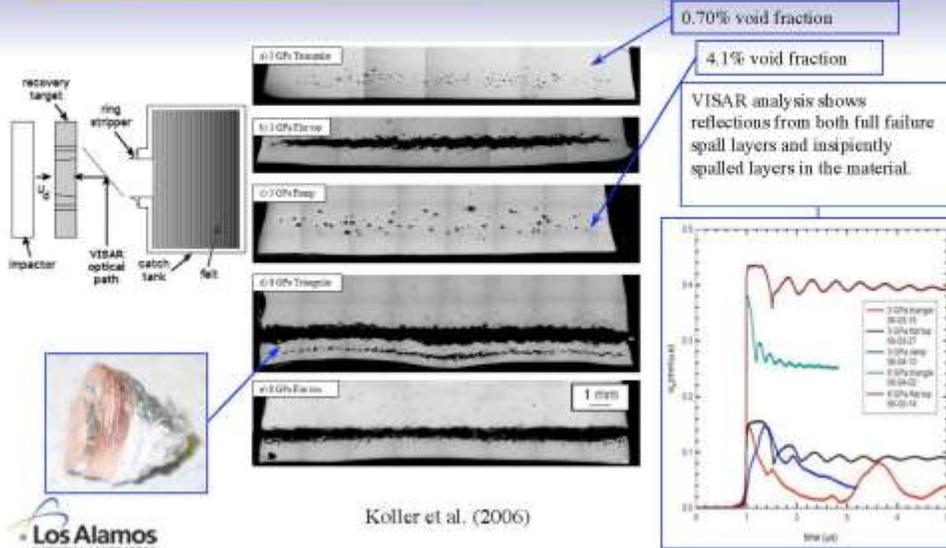
Finally, all available data are used to develop a multi-phase equation of state to describe Zr



- Carl Greeff (T-1) has used all available data to develop and evaluate a multi-phase EOS for Zr.
- Reasonable agreement is obtained between experimental data and simulations for Zr_2 and Zr_1 .
- More work is needed in order to describe the least pure material, Zr_0 .
- This work is helping us understand the influence of impurities and the mechanisms responsible for phase transformations.
- This, and similar work, is helping to develop more accurate equations of state for use in today's hydrocodes.

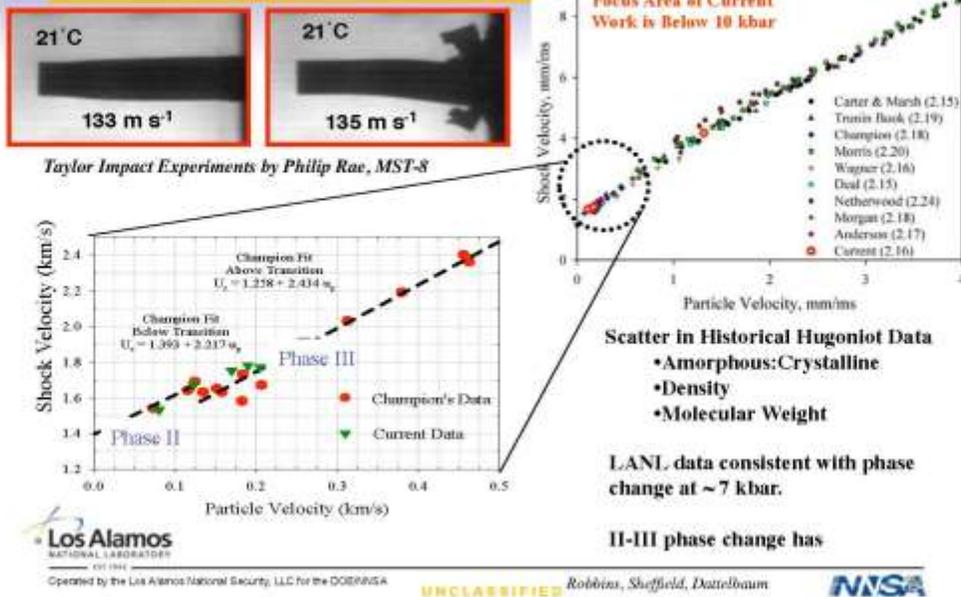
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Recovery experiments with post experiment metallurgical analysis illustrate dependence of dynamically induced damage on shock wave profile shape.



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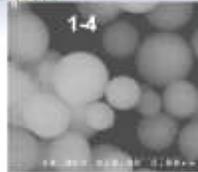
Low pressure phase behavior of PTFE: does the II-III transition occur dynamically?



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Fabrication and characterization of explosive samples is essential to interpreting hot spot effects.

- Gelled with guar at 1.75 – 1.85 wt%



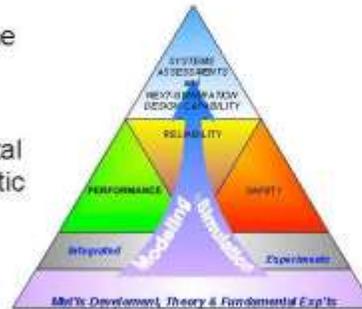
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International Shock Wave Database would provide a useful foundation

- Quality shock wave data provides information to test strength, damage, thermodynamic, and kinetic models.
- As hydrodynamic codes are produced the data would provide for an algorithm validation suite.
- The database could assist in experimental design or assist in proofing new diagnostic techniques as they become available.
- Provide the engineers with validated material models



International Shock Wave Database – Logistic thoughts

- Shock wave data requires a bit of analysis
 - Information on which window correction used
 - Information on the configuration and pedigree of the shot
 - Accuracy of the data technique
- Assuming that the data could be shared, promoting the academic sharing of data beyond what may be publication ready
- Recognizing that there are potential errors that could crop up from the technique used and interpretation of data

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The Perspective from LLNL
Presented at the International Shock-Wave
Database Workshop (ISWdb)
GSI-FAIR, Darmstadt, Germany



Mukul Kumar

Condensed Matter & Materials Division

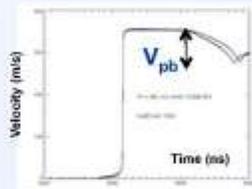
This work was performed under the auspices of the U.S. DOE by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

At LLNL we employ a variety of methods

- The techniques range from diamond anvil cell (both at LLNL and Advanced Photo Source), gas guns (LLNL and CalTech), laser methods (LLNL-JANUSP, Omega), and pulsed power methods (SNL)
- Static pressure measurements and shock measurements complement each other
- Ramp compression methods are starting to come on-line, but highlight limitations in any method where plastic dissipation cannot be ignored

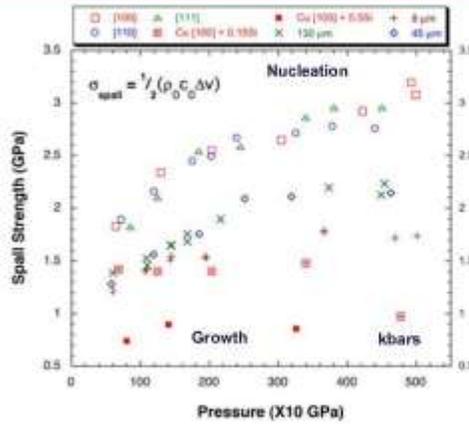


The influence of microstructure on spall is quantified by analyzing pullback velocities from gas gun shots



With increase in density of potential void nucleation sites, there is a transition from nucleation limited regime for single crystals to growth dominated (easy nucleation) response in "dirty" microstructures

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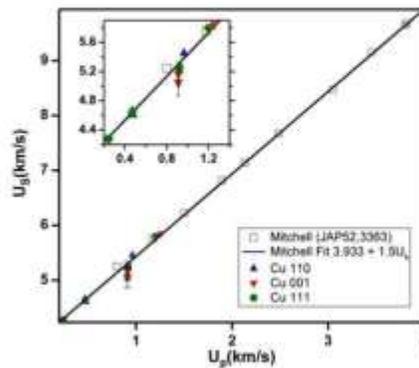
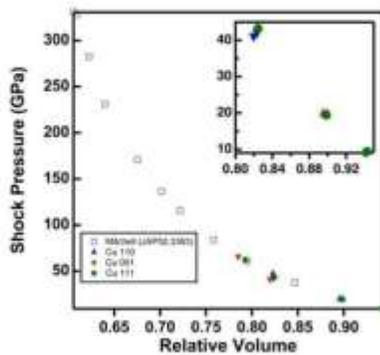


Minich, Cazamias, Kumar, Schwartz;
Metallurgical & Materials Transactions, vol. 35A, p. 2663 (2004)



3

Measurements to extract EOS may be "colored" by plasticity and other anisotropic materials effects



Chau et. al., Journal of Applied Physics, vol 107, Iss 2 (2010)

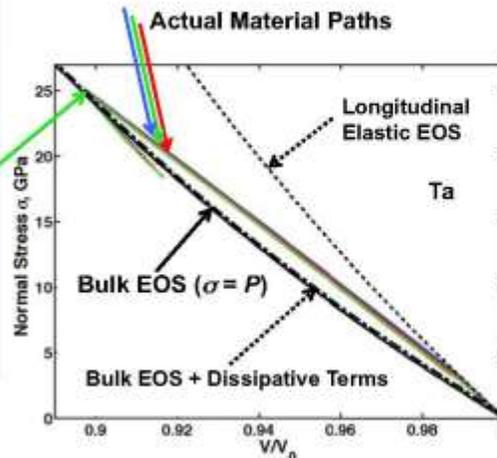
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4

When high precision is required, the distinction between pressure and normal stress is very important

- Strength information is calculated from difference between material paths and EOS paths
- If the EOS mistakenly includes strength, the calculated strength *here* is essentially zero
- Many EOS's from dynamic experiments include strength implicitly and make no distinction between σ and P
- If we truly want 1% precision, our databases *cannot* have problems like this



Reed et. al., *Journal of Applied Physics*, in press (2011)

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Several issues have to be addressed in order to have an effective database

- What is the provenance of the data?
- What are the assumptions in extracting useful information from the raw data and how much data "massaging" is required or acceptable?
- How do we represent and present the data?
- The issue at hand is not unlike what is being faced by the community that is looking into climate change (on a much bigger scale, of course)
- An independent effort (Berkeley Earth Surface Temperature) has been started, which includes recent Nobel prize winners and other high profile scientists who are not necessarily climatologists
- Their website, <http://berkeleyearth.org/>, promises a transparent approach, which is Independent, Replicable & Inclusive (their words)

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Things we like about the existing database (with input from Phil Sterne and the LLNL EOS group)

- **Web-based – wide accessibility and easy to use**
- **Comprehensive datasets – all source data-points are represented; does not “sample representative points” for large datasets**
- **Ability to down-select to set of materials of interest**
- **Well-documented reference to original source material**
- **Plotting capability offers a quick review of regions spanned by data**

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Improvements we would like to see

- **Retain original source data values, i.e. no rescaling for “consistency”**
 - Offer consistently rescaled data only upon user request
 - Ideally store data in original units for ease of comparison with original sources and convert to user-selected unit system on request
- **Extend database to include more recent data**
 - Including laser-driven shock data, Z-pinch data...
- **Add related thermodynamic data sources**
 - e.g., DAC data, isobaric data, melt curves...
- **Provide a more flexible search and data-selection user interface**
 - e.g. global search for all materials containing Al and Ti
 - Sub-selection, e.g. narrow search results to gas-gun-only, or oxides only, or post-1980 only, or citations by Trunin only, or...
- **Offer more interactive plotting capabilities**
 - Click on data point to identify data value and source
 - Overlay user-provided experimental data and/or analytic or tabular theory curve
- **Offer XML output in addition to tabular ASCII form**

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Desired thermodynamic data

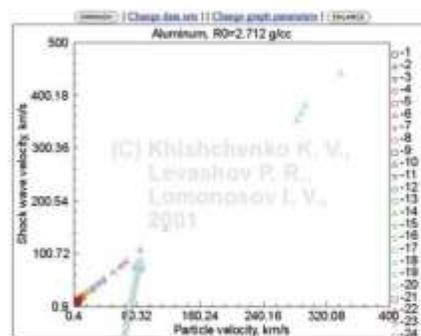
- Hugoniot
- Porous Media
- Shock Release data
- Diamond Anvil Cell Isotherms
- Isobaric and Isochoric trajectories
- Adiabats
- Melt Curves

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Desired data format and user interface features

- Host experimental data in the format that is consistent with the original publication/source
- Provide direct link/access to the original publication/source
- If the original data has been scaled or changed in any fashion, alert users and post the details of transformation
- Provide flexibility in data formats and unit conversions



Direct link to data by clicking on symbols on graphs

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Material Implementation Database & Analysis Source (MIDAS)

Meijie Tang and team

- Placeholder to upload/download experimental data and references (*share/store/manage*)
- Database for 'blessed' model and model parameters (*share/store*)
- Easy curve fitting and comparison with experimental data (*view/manipulate*)
- Central source code for material model implementations (*implement*)
- Web-based access with access controls (*community resource*)
- Enable hydro-codes to initialize material properties from a single database repository (*deploy*)

MIDAS Goal: Build a central repository and its enabling software platform

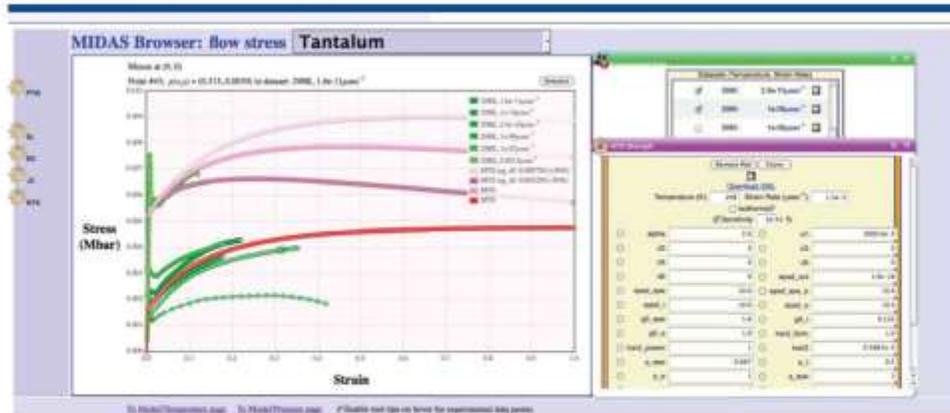
MIDAS Functions: Share, store, view, manage, implement, and deploy material properties

MIDAS Databases: Use xml format, central repository for experimental data, model parameters database are releasable

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MIDAS browser alpha0.1: snapshot



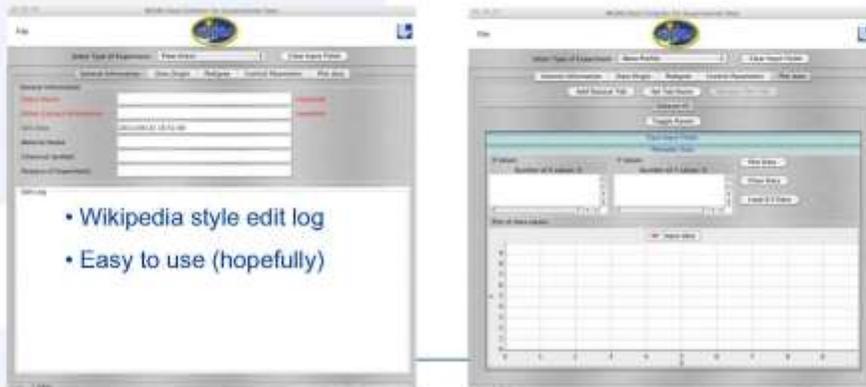
MIDAS web browser: Users can view experimental data, model fits, and documentation; Also compare model fits with experimental data and manipulate parameters interactively

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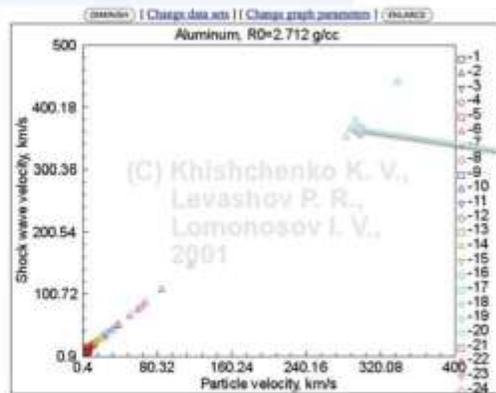
MIDAS experimental data collector (Peter Norquist)

- Types of data: flow stress, wave profile, others
- Types of experiments: gas gun, Z, HE driven, Laser driven
- Thorough documentation: contact, reference, date
- Data upload formats: CVS, whitespace, Excel, paste; download to xml format
- Instantaneous plotting and viewing



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Desired user interface features



Direct link to data by clicking on symbols on graphs

Database Design Issues

ISWdb workshop

Ralph Menikoff

Key design issues

- **Intended audience**
User base
- **Data entry**
Experimentalist or database staff
- **Future extensions**
Numerical experiments such as molecular dynamics

Affects structure of database

- What data to include**
- Format of data files**
- Long term support**
Serve needs of user base

Example of database design – HED

High Explosive Database

C. Scovel & R. Menikoff

Aimed at small scale HE experiments

Experimental data rather than handbook properties

■ **Intended Audience**

- HE modelers
Design & calibrate models
- Verification & Validation community
Data to compare with simulations
- Experimentalists
Archive experimental data

Funding from user community sponsors

ISWdb

Thermodynamic & mechanical
Properties of materials

- EOS models
high pressure regime
- Strength models
elastic-plastic waves
failure waves

HED – Types of data

■ **Overdriven detonation locus**

EOS of reactants – shock Hugoniot data

■ **Profile data**

- VISAR, PDV
impedance mismatch with window
- Embedded velocity gauges
Lagrangian time history
Raw vs. reduced vs. processed data

■ **Digitized image**

Streak camera record
Radiograph

Variety of data types

Need flexible data file format

ISWdb

- Thermodynamics – EOS
Loci are curves in phase space
– shock locus
– release isentrope
Sample more of phase space
– vary initial state for loci
Phase transitions
– sound speed behind shock
Decomposition in plastics
– "kink" or bend in shock locus
– approach to equilibrium
- Mechanical properties
Plastic waves profiles
Time dependent phenomena
– rate effects
– multiple gauges per experiment

HED – Database structure

■ Characterize HE

Initial density and temperature
– Affects detonation properties
Lot of very similar experiments

■ Entry by experiment

Shot number to identify experiment
Brief description of experiment
Links to published papers
Multiple data file attachments
Plot files of data

Find specific data set

Database needs good search capability
Tags and keywords

Rusbank shock wave database

- Material
- Shock locus or release isentrope table of points
 - multiple experiments / locus
 - Allow for other types of data ?
 - off principal locus
 - time dependent plastic waves
 - Sensitivity and characterization
 - dislocation density
 - grain size



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Slide 5

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HED – Data format

■ Flexible data file format

- Different types of experiments
- Different types of diagnostics
- Possibly multiple diagnostics for single experiment

■ Data file header

- Key experimental parameters
- Easy to parse – automate V & V simulations

■ Long lived

- Standard open formats
 - text, pdf, jpg, . . .
- Other open formats
 - spread sheets, mathematica notebook, . . .
- Proprietary formats
 - commercial plotting software

Trade-Off

- Restrict data types
- More rigid format
- Interactive plotting



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Slide 6

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HED – Data entry

■ New experiments

- Experimentalist
 - File format not too rigid
- WEB based data entry
 - Entry procedure not too burdensome
- Work flow
 - Entry/Review procedure
 - similar to paper submission for journal
 - National labs – need to ensure unclassified data

■ Old experiments

- From literature
 - Scan profile plots, loss accuracy
- Lab records or experimentalists' computer
 - Need to fully specify experiment for simulation

Trade-Off

- ISWdb staff enters data
 - control format of data
 - standardize units
- Profile data
 - scanned data
 - may not be accurate
 - experimental details
 - may be missing

Abstract

Constraining equation of state theory to experimental and theoretical data

Scott Crockett

The purpose of this talk is to highlight the experimental and theoretical data used for generating equation of state. The experimental data shown in the talk is just a subset of data one would wish to find in a centralized web archive.



T-1 PHYSICS AND CHEMISTRY OF MATERIALS
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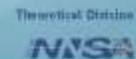


Constraining equation of state theory to experimental and theoretical data

Scott Crockett, T-1
Los Alamos National Laboratory

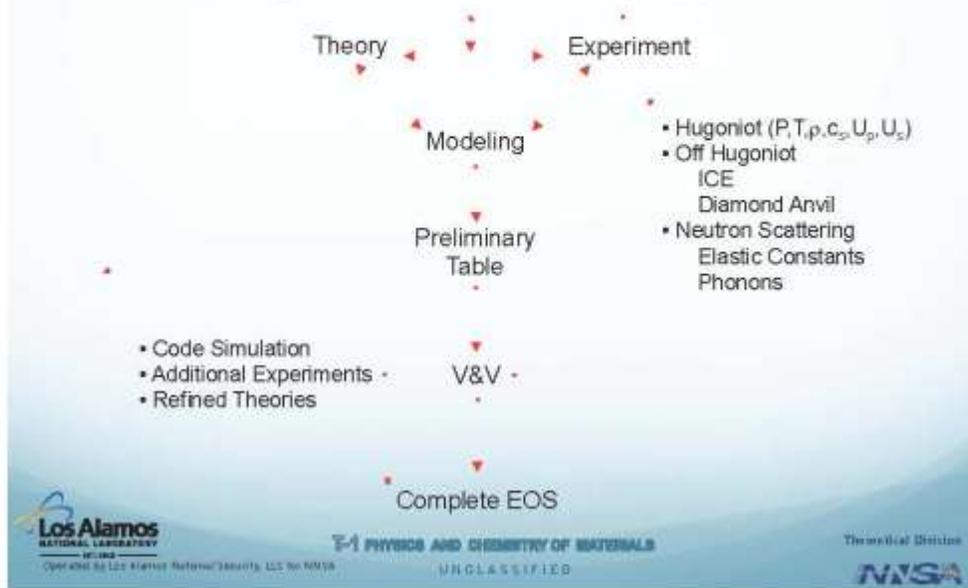


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Equation of State

Making an EOS: Technical Approach



Theoretically Derived Data

- DFT - Density Functional Theory
- Phonons
- Phase transition predictions
- OFMD – Orbital Free Molecular Dynamics
- QMD – Quantum Molecular Dynamics

Experimentally Measured Data

- Near-ambient Pressure Data
 - Density
 - Melt and Boiling Point
 - Thermal expansion
 - Acoustic Data
 - Specific Heat
 - Phonon / Elastic Moduli
 - Isobaric

Experimentally Measured Data

- High Pressure Data
 - Melt Curve
 - Shock
 - Diamond Anvil
 - Phonon/Elastic Moduli
- Other Data
 - Vapor curve
 - Critical Point

Near-ambient Pressure and Other Data Source

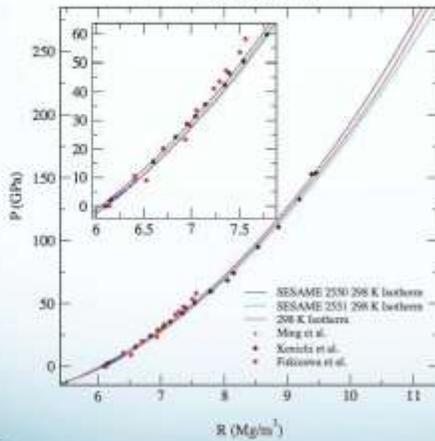
- Solid State Physics (Kittel)
- CRC Handbook of Chemistry and Physics
- Solid State Physics, Vol. 16 1964 (Gschneidner)
- Thermodynamic Properties of the Elements (Hultgren)
- Phase Diagrams of the Elements (Young)
- D. Wallace's Book
- SCCM proceedings
- General Literature Search (no special source generally used)
- When in doubt ask your friendly neighborhood experimentalist (WX-9, etc.)

High Pressure Data

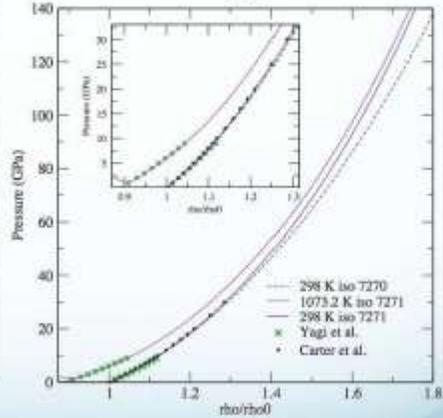
- ✓ Diamond Anvil
- ✓ Melt
- ✓ Shock Hugoniot

Diamond Anvil Examples...

Vanadium



LiF



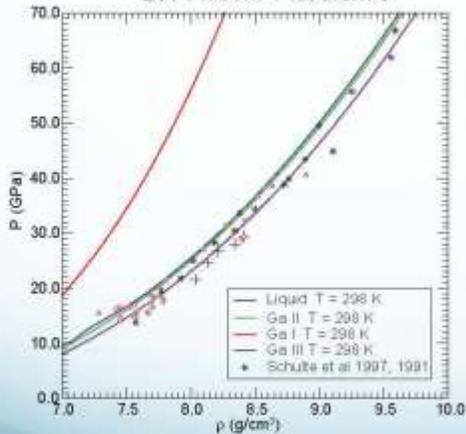
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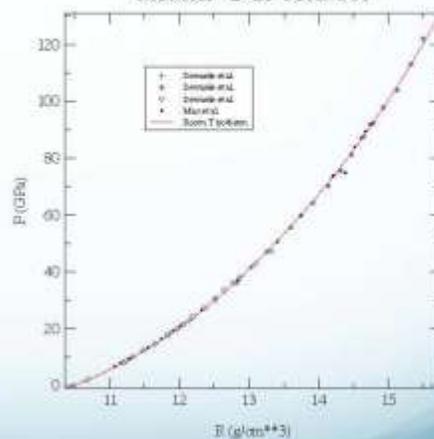
Theoretical Division
 NNSA

Diamond Anvil Examples...

Gallium
2371 Room T isotherms



Silver
Material 2721 Table 301



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T-1 PHYSICS AND CHEMISTRY OF MATERIALS
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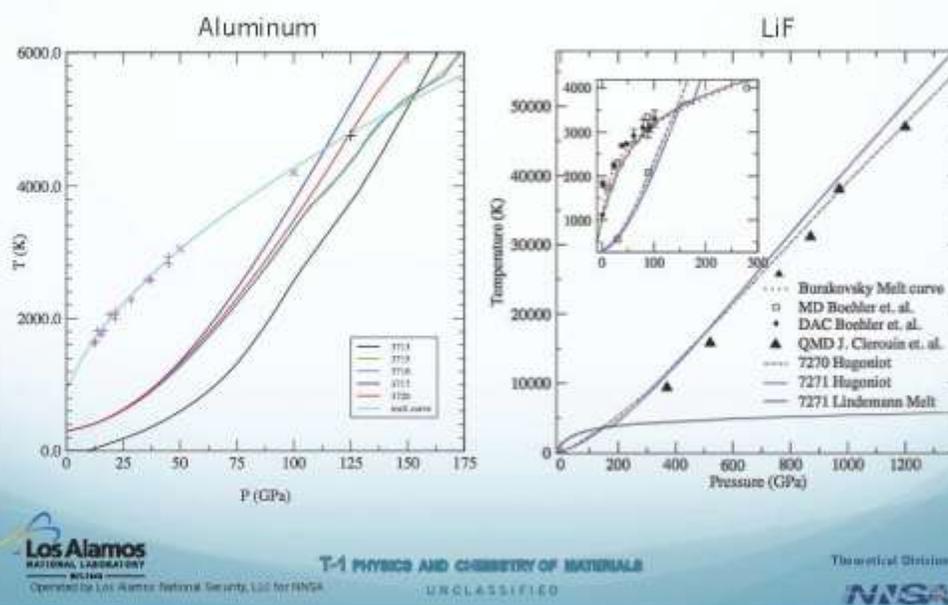
Theoretical Division
 NNSA

Diamond Anvil Data Source

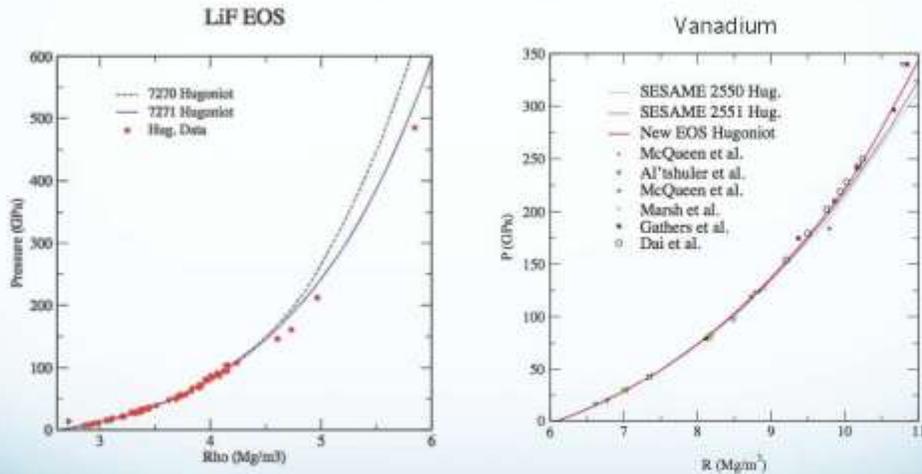
- ✓SCCM proceedings
- ✓General Literature Search (no special source generally used)
- ✓When in doubt ask your friendly neighborhood experimentalist (WX-9, etc.)



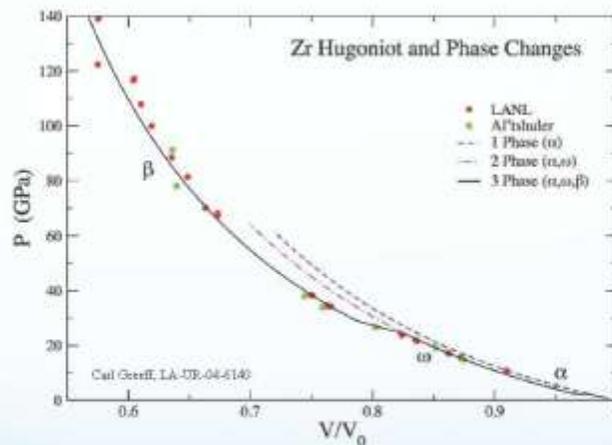
Melt Data ...



Examples of Hugoniot Data

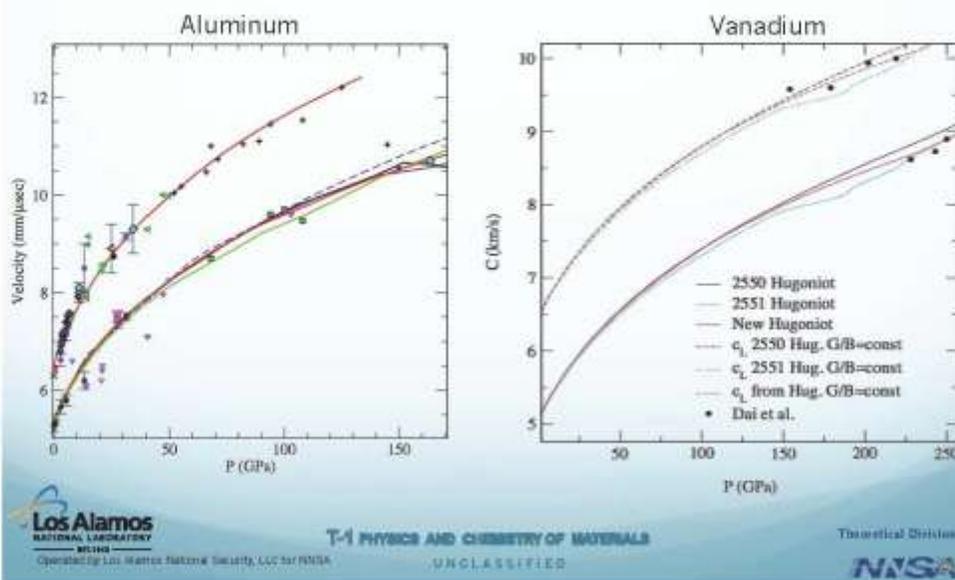


Multiphase Hugoniot

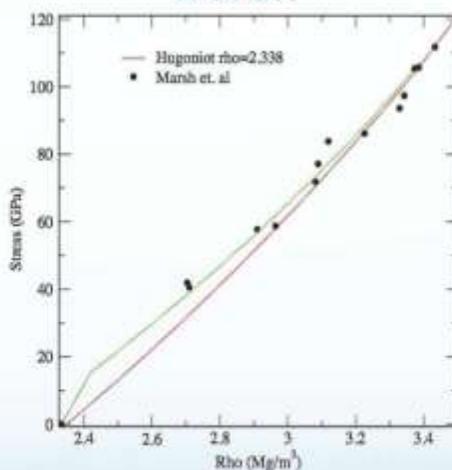


What are the details with regards to wave splitting?
Are the jump conditions solve correctly?

Sound speed under shock compression ...



Strength Effects under Shock Loading ... Boron

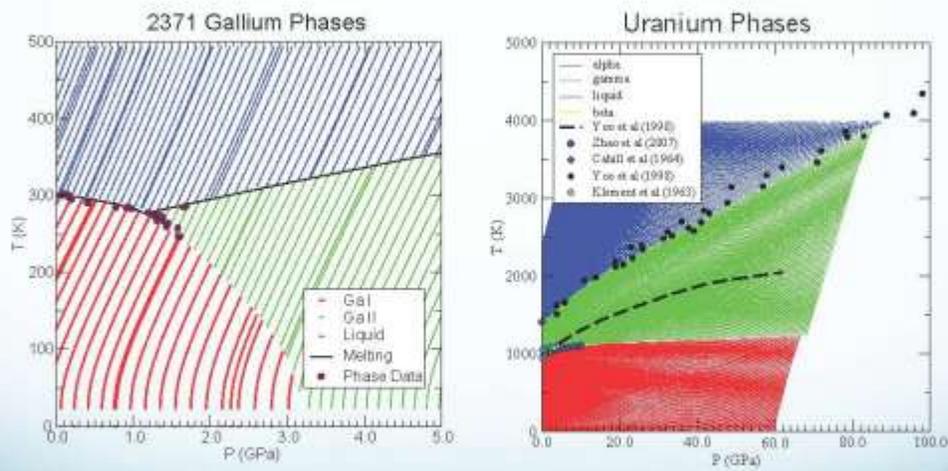


What was actually measured? Measurement techniques need to be documented.

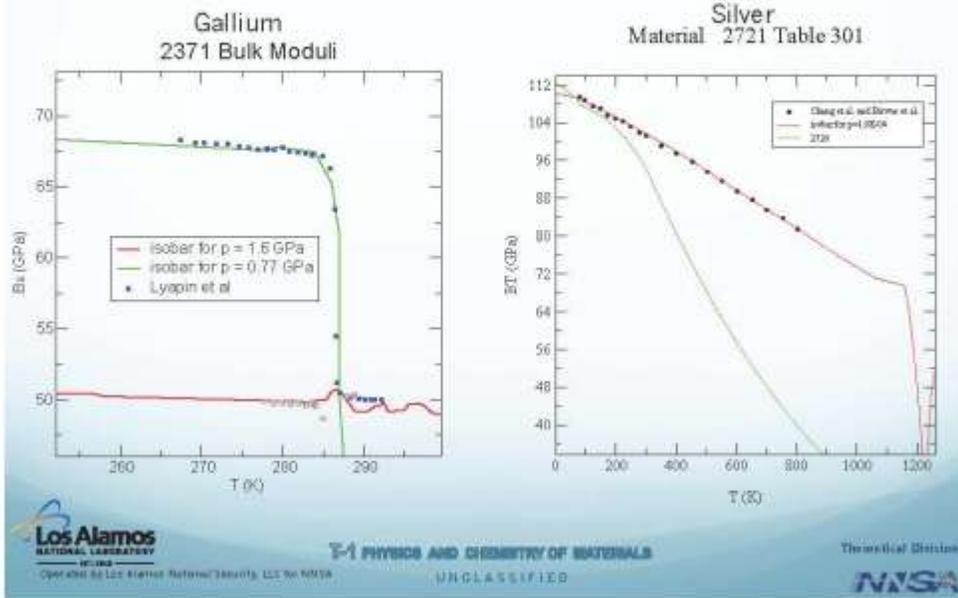
Hugoniot Data Sources

- LASL Shock Hugoniot Data (Marsh)
- Compendium of Shock Wave Data (M. Van Thiel)
- Experimental Data on Shock Compression and Adiabatic Expansion of Condensed Matter (R. F. Trunin)
- <http://teos.ficp.ac.ru>
- SCCM proceedings
- General Literature Search
- When in doubt ask your friendly neighborhood experimentalist (WX-9, etc.)

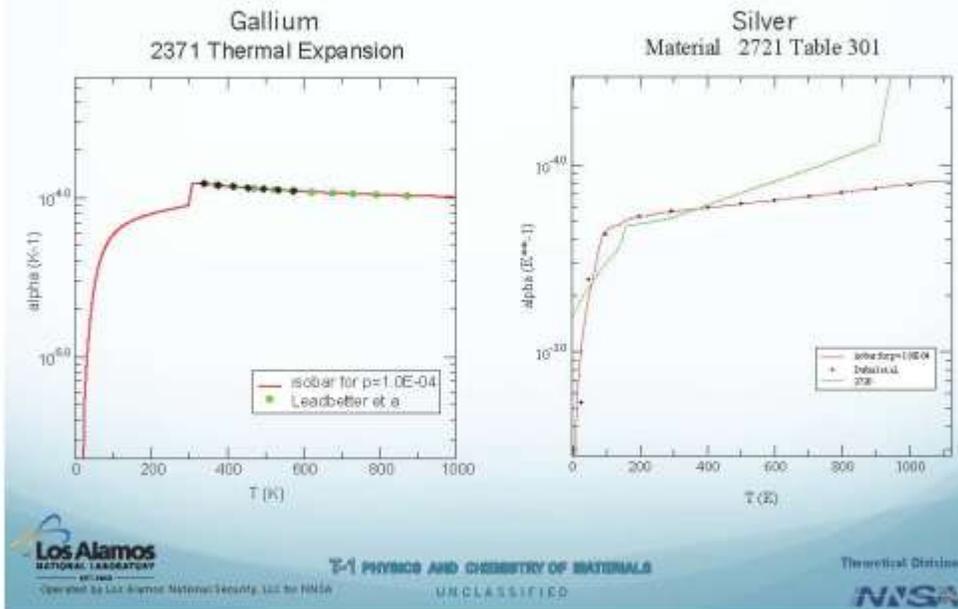
Phase Boundary Data



Isobaric Data



Isobaric Data



DISTRIBUTION

Electronic Distribution:

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