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ON

"PHYSICS OF CONDENSED MATTER AT PLANETARY PRESSURES"

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SHOCK WAVE EXPERIMENTS AND THEIR INTERPRETATION

W.J. NELLIS

Lawrence Livermore National Laboratory
Livermore, California 94550
U.S.A.

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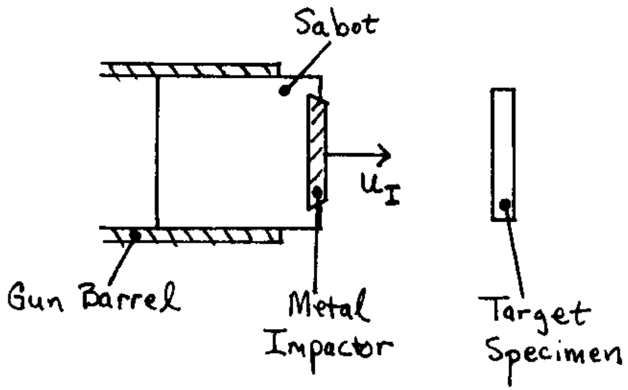
INTRODUCTION

EXTREME CONDITIONS HAVE BEEN ACHIEVED IN CONDENSED MATTER USING CHEMICAL EXPLOSIVES, HYPERVELOCITY GUNS, AND NUCLEAR EXPLOSIVES.

CONSIDER A GUN-LAUNCHED PROJECTILE WHICH GENERATES A SHOCK WAVE BY IMPACT:



Initial State

P_0 E_0

V_0 T_0

$P_0 = P(V_0, E_0)$

PLANAR PROJECTILES CAN BE ACCELERATED TO 8 KM/S BY LIGHT-GAS GUNS. ON IMPACT THE SURFACE LAYERS ARE COMPRESSED AND WORK IS DONE ON BOTH IMPACTOR AND TARGET. THIS PROCESS GENERATES A DYNAMIC PRESSURE: $P_0 \rightarrow P(V_0 - \Delta V, E_0 + \Delta E) > P_0$.

THE TWO-STAGE LIGHT-GAS GUN AT THE LAWRENCE LIVER NATIONAL LABORATORY IS ILLUSTRATED:

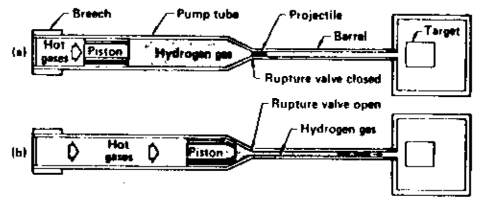


FIG. 6. Schematic diagram of the Lawrence Livermore National Laboratory two-stage, light-gas gun. The pump tube is 10 m long and the barrel or launch tube is 9 m long.

THE GUN IS DESCRIBED BY JONES, et al, 1966. IT CONSISTS OF A BREECH CONTAING A FEW KG's OF GUNPOWDER (FIRST-STAGE DRIVING MEDIUM), A PUMP TUBE FILLED TYPICALLY WITH 60g of H_2 GAS (SECOND-STAGE DRIVING MEDIUM), AND AN EVACUATED, SMOOTH-BORE LAUNCH TUBE. HOT GASES FROM THE BURND GUNPOWDER DRIVE A 6 KG PISTON INTO THE PUMP TUBE, COMPRESSING THE H_2. WHEN THE GAS IS COMPRESSED TO A PRESSURE OF ABOUT 1 KBAR, THE RUPTURE VALVE OPENS AND THE COMPRESSED GAS ACCELERATER THE PROJECTILE. THE PUMP TUBE AND LAUNCH TUBE OR BARREL HAVE INNER DIAMETERS OF 90 AND 28 mm, RESPECTIVELY. THE HIGH VELOCITY IS ACHIEVED BY THE INCREASED SOUND VELOCITY OF THE GAS AT THE HIGHER TEMPERATURE ACHIEVED BY ISENTROPIC COMPRESSION IN THE PUMP TUBE AND BY ROUGHLY CONSTANT MASS

FLOW RATE OF THE GAS THROUGH THE TAPERED SECTION. H_2 IS USED BECAUSE IT PRODUCES THE HIGHEST SOUND VELOCITIES AND HIGHEST MUZZLE VELOCITIES. THE SOUND VELOCITY IN THE GAS DETERMINSES THE MAXIMUM RATE AT WHICH THE GAS CAN TRANSMIT PRESSURE TO DRIVE THE PROJECTILE. FOR AN IDEAL GAS, WHICH H_2 APPROXIMATES IN THIS APPARATUS, SOUND VELOCITY IS PROPORTIONAL TO $\sqrt{T/M}$, WHERE T IS TEMPERATURE AND M IS MOLECULAR WEIGHT. H_2 HAS THE SMALLEST MOLECULAR WEIGHT OF ANY GAS AND IS COMPRESSIBLE TO HIGH TEMPERATURE BY THE HEAVY PISTON. THE PHYSICAL LIMITS TO PROJECTILE VELOCITY ARE THE SOUND VELOCITY OF THE GAS. PRACTICAL LIMITS ARE THE STRESSES IN THE TAPERED SECTION AND THE BREECH.

EXAMPLES OF SINGLE-SHOCK COMPRESSION

MATERIAL	SHOCK PRESSURE (Mbar)	SHOCK COMPRESSION
Liquid D_2	0.2	3
SiO_2	1-20	2+
Fe	9+	2+

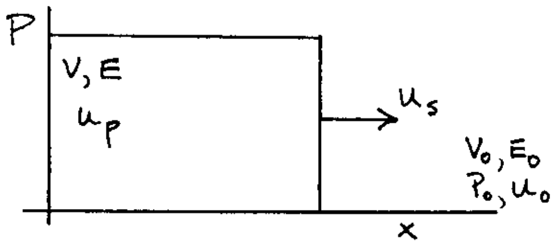
TEMPERATURES WERE > 5000 K

THE SHOCK PROCESS IS SO FAST (~1 μs) THAT THERMAL ENERGY CANNOT BE TRANSPORTED AWAY FROM THE SPECIMEN DURING THE EXPERIMENT. THEREFORE, HIGH TEMPERATURES ARE ACHIEVED.

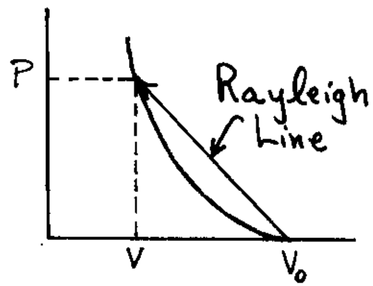
THE CONDITIONS ACHIEVED ARE COMPARABLE TO THOSE IN THE EARTH AND THE OUTER PLANETS.

WHAT IS A SHOCK WAVE ?

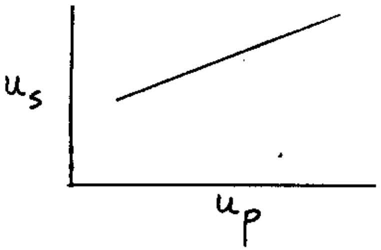
A SHOCK WAVE IS A WAVE IN MATTER WITH A DISCONTINUITY IN FLOW AND THERMODYNAMIC VARIABLES.

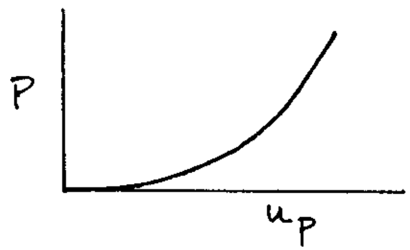


P = PRESSURE
V = VOLUME
E = ENERGY-INTERNAL
u_s = SHOCK VELOCITY
u_p = MASS VELOCITY



LOCUS OF POINTS OF ANY TWO SHOCK PARAMETERS IS CALLED A HUGONIOT CURVE





EQUATION-OF-STATE (P, V, E) DATA ARE OBTAINED FROM SHOCK-WAVE EXPERIMENTS.

MEASURED KINEMATIC PARAMETERS (u_s and u_I) AND INITIAL DENSITIES ARE RELATED TO THESE THERMODYNAMIC VARIABLES VIA THE RANKINE-HUGONIOT EQUATIONS:

$$P = \rho_0 u_s u_p \quad (1)$$

$$V = V_0 \left(1 - \frac{u_p}{u_s}\right) \quad (2)$$

$$E - E_0 = \frac{1}{2}(P + P_0)(V_0 - V) \quad (3)$$

(for specimens initially at rest) and the SHOCK IMPEDANCE MATCH PRINCIPLE:

$$u_p = u_p(u_I, u_s, \rho_0)$$

Note: $V_0 = 1/\rho_0$
$V = 1/\rho$

ARE STATES ACHIEVED BY SHOCK COMPRESSION IN THERMODYNAMIC EQUILIBRIUM?

GENERALLY SPEAKING, YES IN CONDENSED MATTER - BUT NOT ALWAYS.

THERMODYNAMIC EQUILIBRIUM IS ACHIEVED BECAUSE RELAXATION TIMES ARE $\lesssim 10^{12}$ s; FOR EXAMPLE, CONSIDER PHONON FREQUENCIES, ELECTRON-PHONON RELAXATION TIMES, MOLECULAR VIBRATIONAL FREQUENCIES, ETC. SHOCK EXPERIMENTS LAST $\gtrsim 10^{-7}$ s. SO THERE IS SUFFICIENT TIME FOR MANY INTERACTIONS TO ESTABLISH THERMAL EQUILIBRIUM.

MOLECULAR DYNAMICS (KLIMENKO AND DREMIN, 1978) AND CONTINUUM MECHANICS (HOOVER, 1979) SHOW THAT IN DENSE FLUID Ar THE SHOCK WIDTH IS ~10 Å AND FOR A SHOCK VELOCITY OF ~1 KM/S, THE EQUILIBRATION TIME IS 10^{-13} s. THE RESULTS ARE SHOWN BELOW:

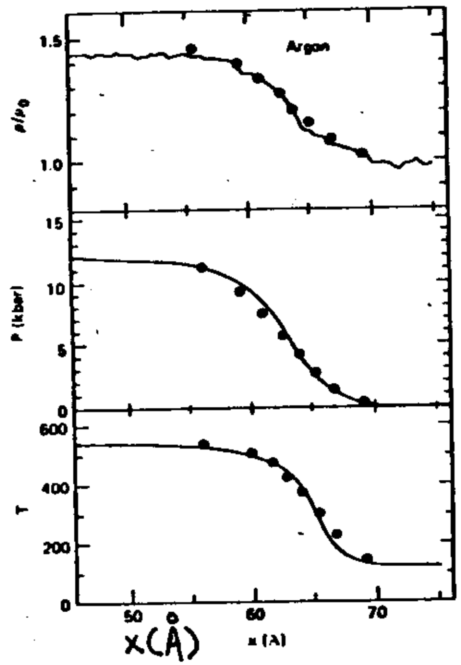


FIG. 2. Density, pressure, and temperature profiles taken from Ref. 1. The full curves are the results from atomistic molecular dynamics. The dots are the present calculations, the solution of the Navier-Stokes equations. Density relative to the initial density, pressure in kilobars, and temperatures in kelvins are given as functions of distance (angstroms). The pressure dots represent the local-thermodynamic-equilibrium pressure. The full curves include, from the Navier-Stokes viewpoint, the bulk-viscosity contribution to the mean pressure. The data shown correspond to a shock velocity of 1.8 km/sec.

SIMILAR THEORETICAL RESULTS ABOUT NARROW SHOCK FRONTS IN SOLIDS HAVE BEEN OBTAINED (HOLIAN AND STRAUB, 1979). SUCH FAST RISE TIMES HAVE NEVER BEEN MEASURED. RISE TIMES OF SHOCK WAVES OBSERVED OPTICALLY IN SOLIDS FOR PRESSURES >100 KBAR ARE LESS THAN THE TIME RESOLUTION OF THE DETECTION SYSTEM, 10^{-9} s.

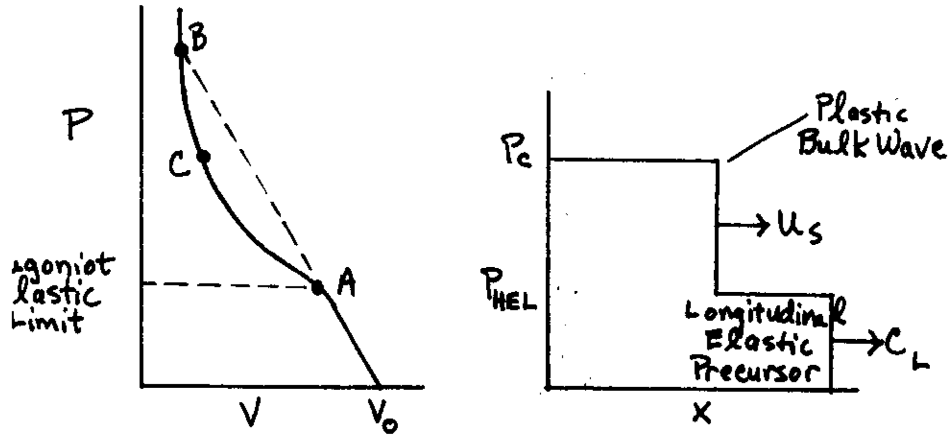
A REASONABLE ESTIMATE OF THE WIDTH OF A STRONG SHOCK WAVE IN CONDENSED MATTER IS 10 - 1000Å, WHICH IS EFFECTIVELY A DISCONTINUITY ON THE SCALE OF THE EXPERIMENTS (mm's).

THERMAL EQUILIBRIUM IS MOST A CONCERN WHEN PROCESSES REQUIRING ACTIVATION ARE INVOLVED: CHEMICAL REACTION AND PHASE CHANGES, FOR EXAMPLE. IF ACTIVATION TIMES ARE LONGER THAN THE EXPERIMENT, THEN EQUILIBRIUM STATES WILL NOT BE ACHIEVED.

SHOCK WAVE STRUCTURE

IN FLUIDS OR IN SOLIDS AT SHOCK PRESSURES WELL ABOVE ELASTIC LIMITS, PHASE TRANSITIONS, ETC., THE SHOCK WAVE STRUCTURE IS A SIMPLE STEP DISCONTINUITY.

IN SOLIDS AT PRESSURES COMPARABLE TO ELASTIC LIMITS OR PHASE-CHANGE PRESSURES, THE SHOCK WAVE CAN HAVE A MULTIPLE WAVE STRUCTURE. CONSIDER AN ELASTIC-PLASTIC SOLID. FOR $P > P_B$ AND $P < P_A = P_{HEL}$, A SINGLE WAVE PROPAGATES. FOR $P_A < P_C < P_B$ - TWO WAVES:

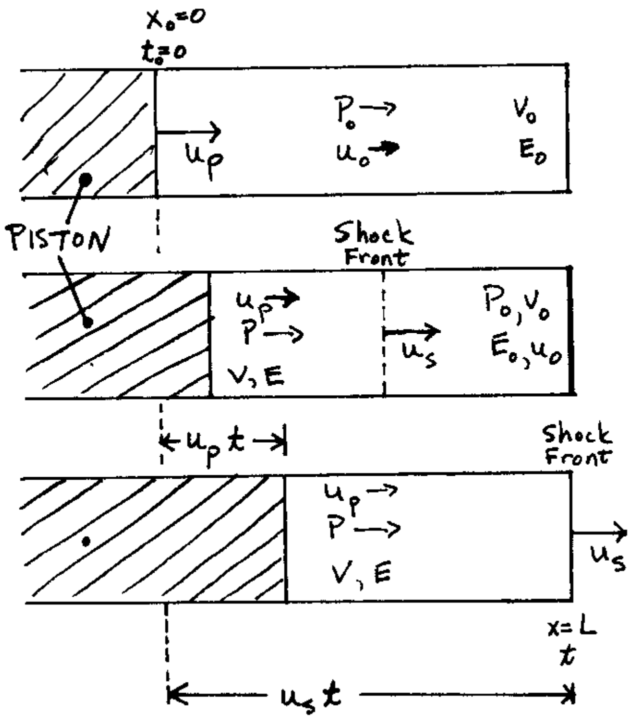


WAVE STRUCTURE MUST BE CONSIDERED WHEN INTERPRETING DATA OR CHOOSING DIAGNOSTICS.

RANKINE–HUGONIOT EQUATIONS

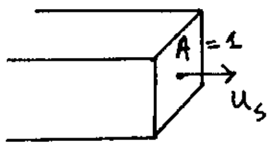
CONSIDER UNIAXIAL FLOW – ONLY IN DIRECTION OF THE SHOCK WAVE.

1. CONSERVE MASS



u_0 and P_0 in same direction. If $u_0=0$, P_0 is scalar.

CONSIDER UNIT AREA



SHOCKED MASS $= \rho_0(u_s-u_0)t = \rho(u_s-u_p)t$ (4)

$$\rho_0(u_s-u_p) = \rho[(u_s-u_0)-(u_p-u_0)] \quad (5)$$

$$\frac{\rho_0}{\rho} = 1 - \frac{(u_p-u_0)}{(u_s-u_0)} = \frac{V}{V_0} \quad (6)$$

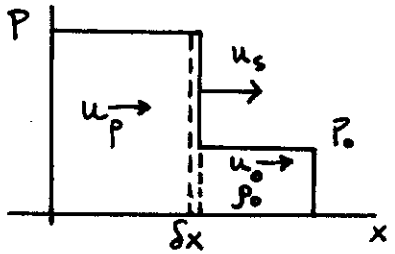
$$\boxed{V = V_0\left[1 - \frac{(u_p-u_0)}{(u_s-u_0)}\right]} \quad (7)$$

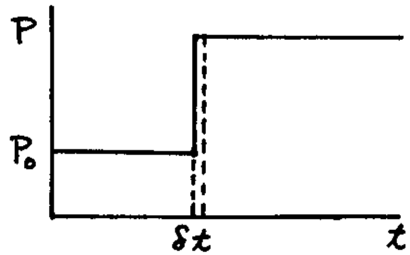
AND

$$(u_s-u_0) = \frac{V_0(u_p-u_0)}{V_0 - V} \quad (8)$$

2. CONSERVE MOMENTUM

$$\int F\,dt = m\,\Delta u$$





MASS SWEPT UP BY SHOCK IN $\delta t = \rho_0 (u_s - u_0)\delta t$

CHANGE IN VELOCITY $= (u_p - u_0)$

$$(P - P_0)\delta t = \rho_0 (u_s - u_0)\delta t\,(u_p - u_0) \qquad (9)$$

$$\boxed{P - P_0 = \rho_0 (u_s - u_0)(u_p - u_0)} \qquad (10)$$

AND

$$\rho_0 (u_s - u_0) = \frac{P - P_0}{u_p - u_0} \qquad (11)$$

DEFINITION: $\rho_0 u_s \equiv$ SHOCK IMPEDANCE

3. CONSERVE ENERGY

NET WORK ON MASS = CHANGE IN TOTAL ENERGY

NET WORK $= P u_p \delta t - P_0 u_0 \delta t$

MASS SWEPT UP IN $\delta t = \rho_0 (u_s - u_0)\delta t$

$$\therefore P u_p \delta t - P_0 u_0 \delta t = \rho_0 (u_s - u_0)\delta t \Big[\underbrace{\tfrac{1}{2}(u_p^2 - u_0^2)}_{\Delta KE} + \underbrace{E - E_0}_{\Delta IE}\Big], \qquad (12)$$

WHERE E AND E_0 ARE THE FINAL AND INITIAL INTERNAL ENERGIES PER UNIT MASS.

$$P u_p - P_0 u_0 = \rho_0 (u_s - u_0)\Big[\tfrac{1}{2}(u_p^2 - u_0^2) + E - E_0\Big] \qquad (13)$$

USING EQUATIONS (8) and (11)

$$P u_p - P_0 u_0 = \frac{P - P_0}{u_p - u_0}\Big[\tfrac{1}{2}(u_p + u_0)(u_p - u_0)\Big] + \frac{\rho_0 V_0 (u_p - u_0)}{V_0 - V}(E - E_0) \qquad (14)$$

$$\tfrac{1}{2}(P + P_0)(u_p - u_0) = \left(\frac{u_p - u_0}{V_0 - V}\right)(E - E_0) \qquad (15)$$

$$\boxed{E - E_0 = \tfrac{1}{2}(P + P_0)(V_0 - V)} \qquad (16)$$

CONSIDER 2 LIMITING CASES.

a) WEAK SHOCKS

$$E = E_0 + \Delta E$$
$$P \simeq P_0$$
$$V = V_0 - |\Delta V|$$

EQ. (16) BECOMES $\Delta E = P_0 |\Delta V|$

HUGONIOT COINCIDES WITH ADIABAT FOR WEAK SHOCKS.

b) STRONG SHOCKS

AS AN EXAMPLE CONSIDER AN IDEAL GAS. THE EQUATION OF STATE IS

$$P = (\gamma - 1)\frac{E}{V}, \quad (17)$$

WHERE $\gamma = C_p/C_V$, THE RATIO OF THE SPECIFIC HEATS. SUBSTITUTE EQ (17) INTO EQ (16) AND SOLVE FOR THE HUGONIOT OF AN IDEAL GAS IN P-V SPACE:

$$\frac{P}{P_0} = \frac{(\gamma+1)V_0 - (\gamma-1)V}{(\gamma+1)V - (\gamma-1)V_0} \quad (18)$$

$P/P_0 \to \infty$ AS $(\gamma+1)V - (\gamma-1)V_0 \to 0$

THUS, THERE IS A LIMITING, MINIMUM HUGONIOT VOLUME

$$V_{MIN} = V_0\left(\frac{\gamma-1}{\gamma+1}\right) \quad (19)$$

AND A MAXIMUM COMPRESSION

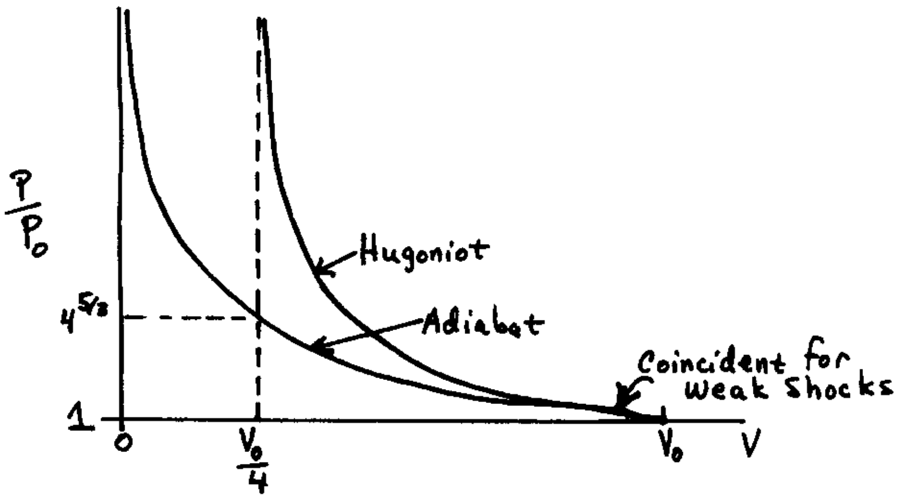
$$\frac{\rho_{MAX}}{\rho_0} = \frac{\gamma+1}{\gamma-1} \quad (20)$$

FOR A MONATOMIC IDEAL GAS $\gamma = 5/3$ AND $\rho_{max}/\rho_0 = 4$.

FOR ADIABATIC COMPRESSION OF AN IDEAL GAS

$$P = P_0\left(\frac{V}{V_0}\right)^{-\gamma} \quad (21)$$

AT $V/V_0 = \frac{1}{4}$ $P/P_0 = 4^{5/3}$.



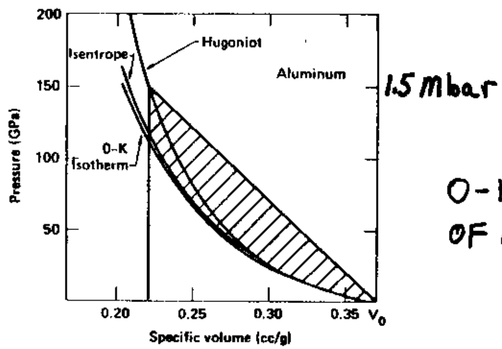
HUGONIOT TEMPERATURE: $\frac{T}{T_0} = \frac{PV}{P_0V_0}$ (22)

NEAR V_{MIN} $T \simeq \left(\frac{T_0}{4P_0}\right)P \Rightarrow T \propto P$

ADIABAT TEMPERATURE: $\frac{T}{T_0} = \left(\frac{P}{P_0}\right)^{\frac{\gamma-1}{\gamma}} \Rightarrow T \propto P^{0.4}$

THE HIGHER TEMPERATURES ACHIEVED AT HIGH SHOCK PRESSURE CAUSE THE LIMITING COMPRESSION.

P-V CURVES FOR ALUMINUM UP TO 1.5 MBAR ARE SHOWN IN THE FOLLOWING:



0-K ISOTHERM OF McMAHAN.

FOR STRONG SHOCKS THE ENERGY EQ. (3) BECOMES

$$E = \frac{1}{2}P(V_0 - V) \quad (23)$$

THUS, THE SPECIFIC INTERNAL ENERGY CAUSED BY SHOCK COMPRESSION FROM V_0 TO V IS THE AREA OF THE TRIANGLE UNDER THE RAYLEIGH LINE. THE ISENTROPIC COMPRESSION PATH IS REVERSIBLE AND THE TEMPERATURE AND THERMAL PRESSURE ALONG THE ISENTROPE ARE LESS THAN ALONG THE HUGONIOT. THE IRREVERSIBLE ENERGY IS REPRE-

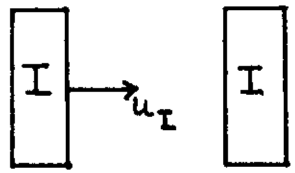
SENTED BY THE SHADED AREA BETWEEN THE RAYLEIGH LINE AND THE ISENTROPE. THIS ENERGY IS AVAILABLE FOR HEAT AND FOR ABSORPTION BY INTERNAL DEGREES OF FREEDOM.

SHOCK IMPEDANCE MATCHING IS A PROCESS USED TO OBTAIN MASS VELOCITY u_p.

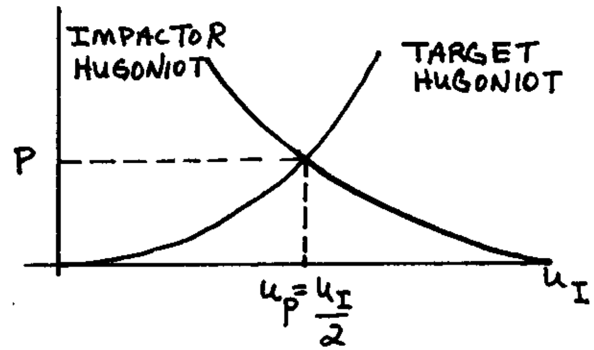
FUNDAMENTAL POSTULATE OF SHOCK-WAVE PHYSICS:

PRESSURE AND MASS VELOCITY ARE CONTINUOUS ACROSS AN INTERFACE BETWEEN TWO MATERIALS

SYMMETRIC IMPACT IS ONE IN WHICH THE IMPACTOR AND TARGET ARE THE SAME MATERIAL:



IN P-u_p SPACE THE COLLISION IS REPRESENTED AS FOLLOWS

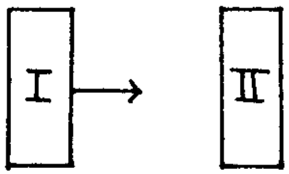


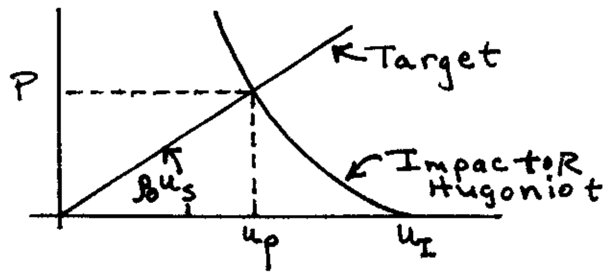
BY SYMMETRY THE MASS VELOCITY $u_p = u_I/2$

BY MEASURING u_I, u_s, AND $\rho_0 = 1/V_0$ THE RANKINE-HUGONIOT EQUATIONS GIVE SHOCK (P, V, E).

EQUATION-OF-STATE STANDARDS ARE DEVELOPED IN THIS WAY—WITHOUT THE NECESSITY OF ANY OTHER PRESSURE CALIBRATION.

<u>NON-SYMMETRIC IMPACT</u> IS ONE IN WHICH IMPACTOR AND TARGET ARE DIFFERENT MATERIALS.





FROM EQ(1) THE STATE IN THE TARGET MUST LIE ON THE STRAIGHT LINE THROUGH THE ORIGIN WITH SLOPE $\rho_0 u_s$ = SHOCK IMPEDANCE. THE IMPACTOR HUGONIOT — MEASURED IN OTHER EXPERIMENTS — IS PLOTTED AS BEFORE. THE INTERSECTION OF THE TWO CURVES IS THE STATE REACHED IN TARGET AND IMPACTOR IN THE COLLISION. THE ANALYTICAL SOLUTION IS OBTAINED:

FOR METALS LIKE THE HUGONIOT STANDARDS AL, CU, AND TA, THE HUGONIOT IS LINEAR IN $u_s - u_p$

$$u_s = C + S u_p , \quad (24)$$

WHERE $C \simeq C_B$, THE BULK SOUND VELOCITY, AND

$$C_B^2 = C_L^2 - \frac{4}{3} C_T^2 , \quad (25)$$

WHERE C_L AND C_T ARE THE LONGITUDINAL AND TRANSVERSE SOUND VELOCITIES AT ZERO PRESSURE.

THEREFORE, u_p IS OBTAINED FROM

$$P = \rho_{0T} u_s u_p = \rho_{0I} [C_I + S_I (u_I - u_p)] (u_I - u_p), \quad (26)$$

WHERE ρ_{0T}, ρ_{0I}, u_I, AND u_s ARE MEASURED IN THE EXPERIMENT AND C_I AND S_I ARE KNOWN FROM PREVIOUS EXPERIMENTS.

DOUBLE-SHOCK EXPERIMENTS

HAVING MEASURED THE HUGONIOT OF A MATERIAL, DOUBLE-SHOCK EXPERIMENTS CAN BE PERFORMED TO ACHIEVE HIGHER PRESSURES AND DENSITIES BUT RELATIVELY LOWER TEMPERATURES. THE SINGLE AND DOUBLE SHOCK CONFIGURATIONS FOR AL ARE SHOWN IN THE FOLLOWING FIGURE (NELLIS, 1983):

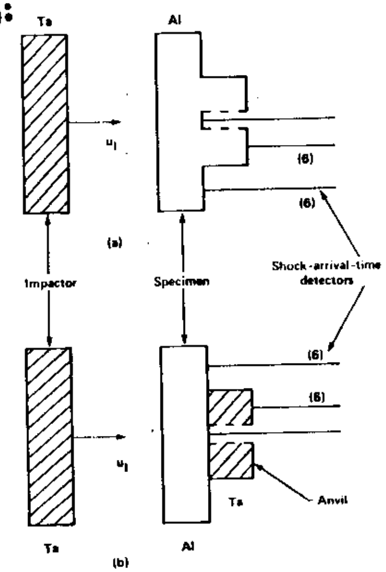
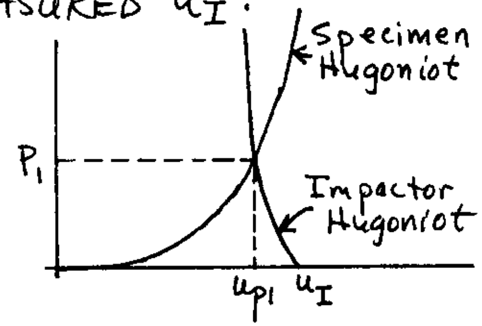


Illustration of (a) a single-shock equation of state experiment and (b) a double-shock equation of state experiment.

FOR THESE EXPERIMENTS THE RANKINE-HUGONIOT EQUATIONS ARE ALSO WRITTEN

SO THAT THE INITIAL STATE IS THE FIRST-SHOCK STATE AND THE FINAL STATE IS THE SECOND SHOCK STATE.

IN GUN EXPERIMENTS THE FIRST-SHOCK STATE IS DETERMINED BY SHOCK-IMPEDANCE MATCHING THE TWO KNOWN HUGONIOTS USING THE MEASURED u_I:



HAVING DETERMINED u_{p1}, THEN u_{s1}, P_1, V_1, AND $E_1 - E_0$ ARE CALCULATED.

THE SECOND SHOCK STATE IS DETERMINED FROM MEASUREMENT OF SHOCK VELOCITY IN THE ANVIL. THEN

$$u_{sAn} = C_{An} + S_{An} u_{p2} \Rightarrow u_{p2} = \frac{u_{sAn} - C_{An}}{S_{An}} \quad (27)$$

THEN $$P_2 = \rho_{oAn} u_{sAn} u_{pAn} \quad (28)$$

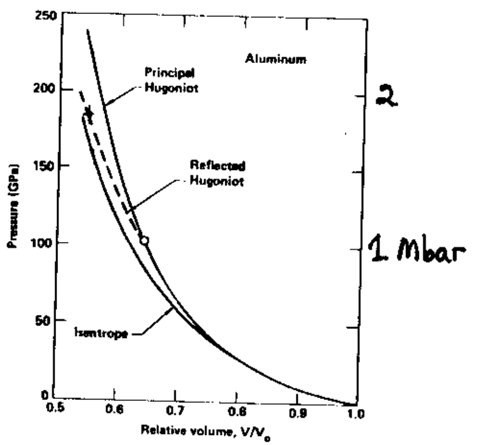
THE DOUBLE-SHOCK VOLUME IS THEN FOUND FROM

$$V_2 = V_1 - \frac{(u_{p_1} - u_{p_2})^2}{P_2 - P_1} \qquad (29)$$

THE DOUBLE SHOCK INTERNAL ENERGY IS OBTAINED FROM SEQUENTIAL APPLICATION OF THE RANKINE-HUGONIOT ENERGY EQ:

$$E_2 - E_0 = (E_1 - E_0) + (E_2 - E_1). \qquad (30)$$

THE RESULT FOR AN AL DOUBLE-SHOCK EXPERIMENT FROM 1.0 TO 1.8 Mbar IS SHOWN:



Double-shock data point for aluminium.[39] The first shock state is represented by the open circle (100 GPa = 1 Mbar).

THE DOUBLE-SHOCK DATA POINT LIES MUCH CLOSER TO THE ISENTROPE THAN TO THE HUGONIOT, A SITUATION FOUND TO BE TRUE GENERALLY.

AS AN EXAMPLE OF DATA, THE FE HUGONIOT DATA IS PLOTTED AS SHOCK VELOCITY VERSUS MASS VELOCITY (FROM BROWN and MC QUEEN, 1982):

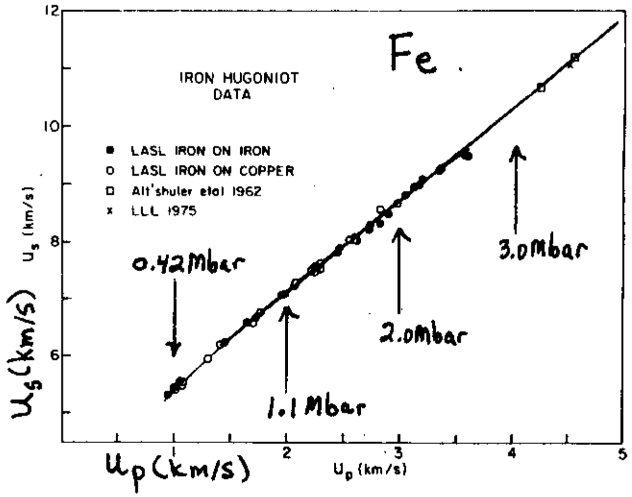
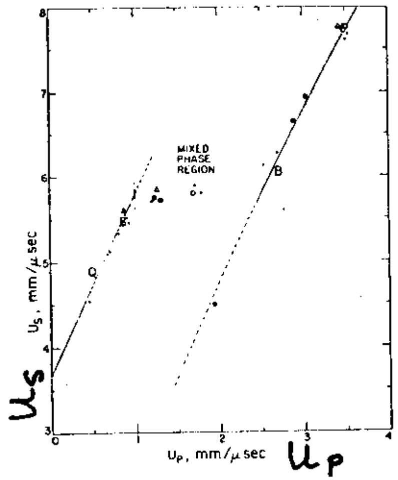


Fig. 3. Selected Hugoniot data for iron. References are (LASL) McQUEEN *et al.*, 1970; AL'TSHULER *et al.*, 1962; and (LLL) MITCHELL, 1975.

THIS DATA FOLLOWS A LINER RELATIONSHIP BETWEEN U_s AND U_p, EQ(24), AS IS COMMON FOR METALS. NO PHASE CHANGES ARE EVIDENT. LATER WE WILL SEE

LATER THAT PHASE CHANGES ARE OBSERVED IN SOUND VELOCITY DATA FOR Fe AT 2.0 AND 2.5 MBAR.

THE u_s-u_p DATA FOR α-QUARTZ (WACKERLE, 1962) ARE SHOWN:



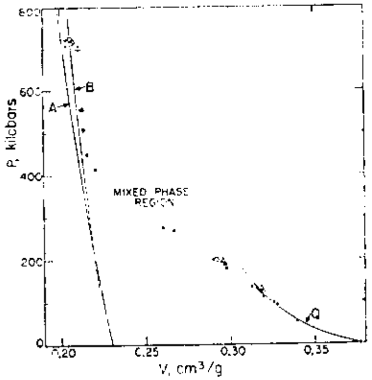
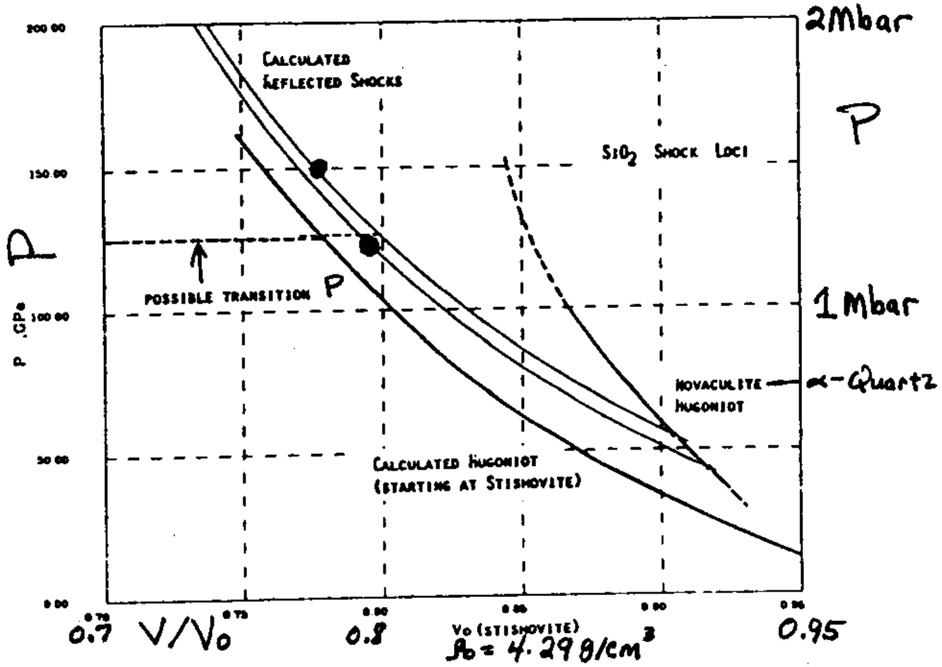


Fig 2. Pressure-volume Hugoniot for crystalline quartz. The points and curves in this figure are the same as in Figure 1; they have been transformed to the P-V plane by the Rankine-Hugoniot equations. Curve A is our best Hugoniot for stishovite with metastable stishovite as the initial condition.

THE SAME DATA PLOTTED AS P-V BY MCQUEEN, FRITZ AND MARSH, 1963, ARE ALSO SHOWN. THE OFFSET IN u_s-u_p REPRESENTS A MIXED-PHASE REGION CAUSED BY THE TRANSITION FROM α-QUARTZ TO STISHOVITE.

DOUBLE-SHOCK DATA FOR α-QUARTZ OF FRITZ AND MC QUEEN ARE SHOWN AS ●:

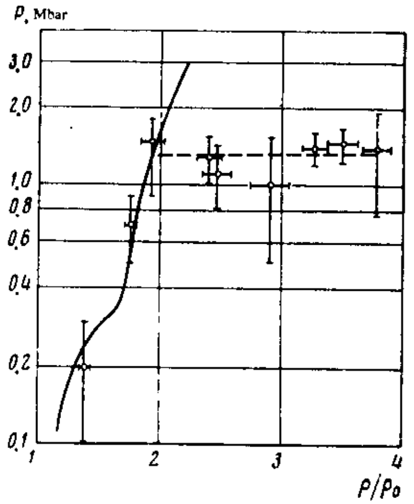


THE DATA AGREE WITH THE CALCULATED DOUBLE-SHOCK (REFLECTED) STATES. NO PHASE CHANGE IS OBSERVED.

THESE DATA WERE OBTAINED TO INVESTIGATE THE COLLAPSE PROPOSED TO OCCUR AT 1.25 MBAR IN α-QUARTZ DURING ISENTROPIC COMPRESSION (PAVLOVSKII et al,

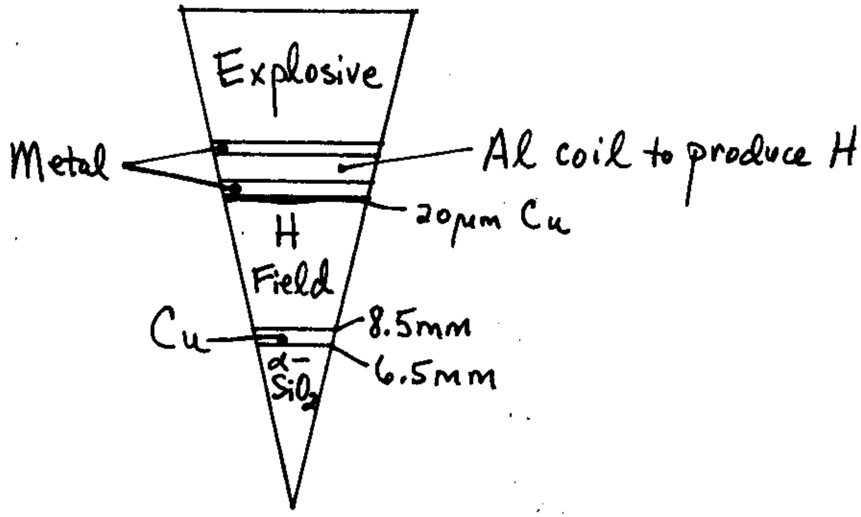
JETP LETT. 27, 265 (1978)). NO PHASE CHANGE IS EVIDENT ON THE α-QUARTZ HUGONIOT AT ~1 MBAR. THESE DOUBLE-SHOCK DATA ARE AT HIGHER DENSITY AND LOWER TEMPERATURE THAN THE HUGONIOT - AND THUS CLOSER TO ISENTROPIC COMPRESSION. BUT NO VOLUME COLLAPSE AT 1.25 MBAR IS OBSERVED. THE POINT AT 1.25 MBAR IS AT THE P-V OF THE ONSET OF THE PROPOSED TRANSITION. THE POINT AT 1.5 MBAR WOULD HAVE TO BE AT 1.25 AND A LOWER RELATIVE VOLUME TO CONFIRM THE TRANSITION.

THE ISENTROPIC-COMPRESSION DATA IS SHOWN HERE. THE SOLID CURVE IS THE HUGONIOT OF α-QUARTZ. THE KINK IS THE STISHOVITE TRANSITION. ABOVE TWO-FOLD COMPRESSION



THE FIGURE SHOWS THAT THE MATERIAL COLLAPSES ANOTHER FACTOR OF 2 IN COMPRESSION. SUCH A LARGE VOLUME COLLAPSE HAS NEVER BEEN OBSERVED IN ANY OTHER SOLID. THE LARGEST KNOWN TO THE AUTHOR IS A ~20% VOLUME CHANGE IN α-QUARTZ AND IN TiO_2.

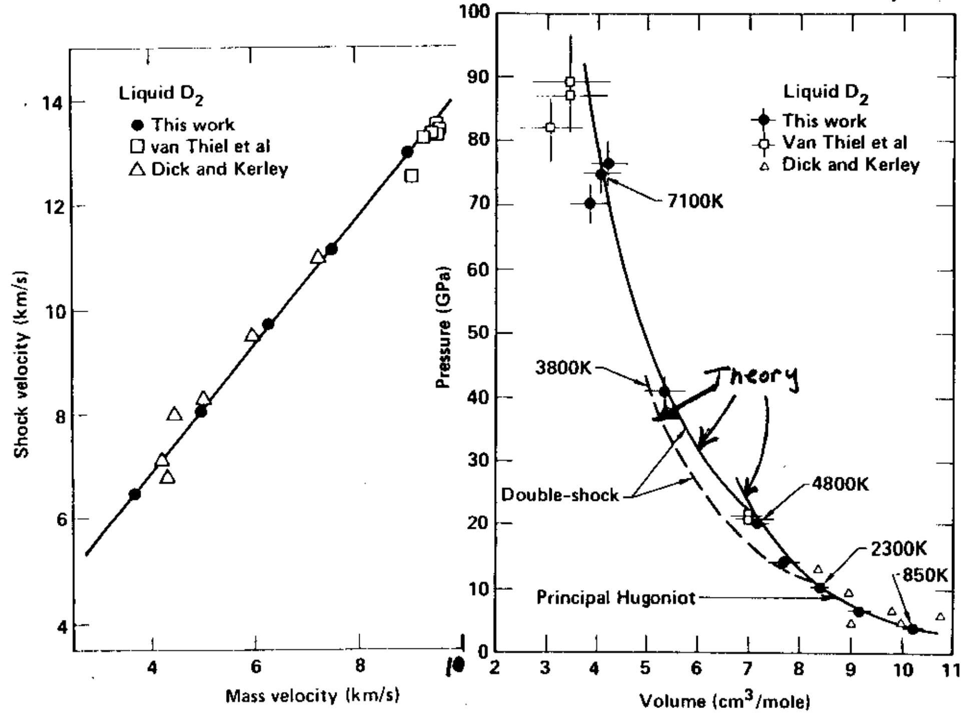
THE CYLINDRICAL SYSTEM USED TO PRODUCE THESE ISENTROPIC COMPRESSIONS IS ILLUSTRATED:



AN INITIAL FIELD OF 100–180 kG IS COMPRESSED TO ~5 MG BY THE EXPLOSIVE, PRODUCING A MAGNETIC PRESSURE OF MORE THAN 1 MBAR. VOLUME IS OBTAINED BY FLASH X-RADIOGRAPHY. PRESSURE IS CALCULATED BY USING THE COMPRESSION AT THE TIME OF THE FLASH X-RAY AND THE KNOWN EQUATION OF STATE OF THE Cu TUBE. THE ASSUMPTION IS MADE THAT THE PRESSURE AND DENSITY ARE UNIFORM OVER THE SAMPLE AND TUBE.

I BELIEVE THIS OBSERVATION REQUIRES INDEPENDENT EXPERIMENTAL CONFIRMATION BECAUSE OF THE ANOMALOUSLY LARGE VOLUME COLLAPSE REPORTED AND THE ABSENCE TO DATE OF EVIDENCE FROM OTHER EXPERIMENTS AT COMPARABLE PRESSURES AND DENSITIES.

ANOTHER EXAMPLE IS THE EQUATION OF STATE OF HYDROGEN. SINCE $P = \rho_0 u_s u_p$ and SINCE THE DENSITY OF LIQUID D_2 IS MORE THAN TWICE THAT OF LIQUID H_2, D_2 SPECIMENS WERE USED TO ACHIEVE ABOUT TWICE THE PRESSURE RELATIVE TO LIQUID H_2 SPECIMENS. THE SINGLE-SHOCK HUGONIOT DATA ARE PLOTTED AS u_s-u_p:



OUR LATEST DATA (NELLIS et al, 1983) SHOW THAT A LINEAR u_s-u_p RELATION IS FOLLOWED. THE DOUBLE-SHOCK DATA ARE ALSO SHOWN. THE CURVES ARE

THEORY (ROSS et al, 1983). THE TEMPERATURES ARE CALCULATED AND HAVE NOT YET BEEN MEASURED.

GRUNEISEN EQUATION OF STATE

WE WILL NOW CONSTRUCT A $P(V,E)$-EQUATION OF STATE USING HUGONIOT DATA AND OFF-HUGONIOT DATA LIKE DOUBLE-SHOCK DATA.

BASIC ASSUMPTION: AT CONSTANT VOLUME

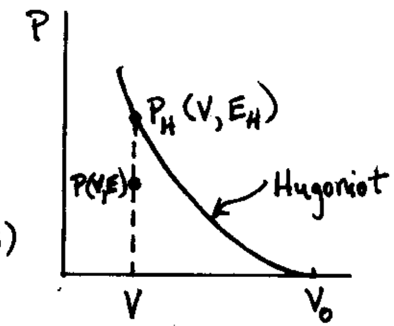
$$\left(\frac{\partial P}{\partial E}\right)_V = \text{CONSTANT} \qquad (31)$$

DEFINE $\gamma \equiv$ GRUNEISEN PARAMETER TO BE A FUNCTION ONLY OF VOLUME

$$(32) \qquad \gamma = V\left(\frac{\partial P}{\partial E}\right)_V$$

THEN

$$\frac{\gamma}{V} = \frac{P - P_H}{E - E_H} \qquad (33)$$



WITH THE HUGONIOT AS A REFERENCE CURVE AND $\gamma(V)$ STATES OFF THE HUGONIOT CAN BE CALCULATED

FROM EQ (33)

$$P = P_H + \frac{\gamma}{V}(E - E_H) \qquad (34)$$

FROM EQ(2)

$$\frac{V}{V_0} = 1 - \frac{u_p}{u_s} \Rightarrow \frac{\rho}{\rho_0} = \frac{u_s}{u_s - u_p} \qquad (35)$$

DEFINE $\eta = \rho/\rho_0 \qquad \mu = \eta - 1 \qquad (36)$

$$u_s = C + S u_p$$

EQ (35) BECOMES

$$\frac{C + S u_p}{C + S u_p - u_p} = \eta = \mu + 1 \qquad (37)$$

$$u_p = \frac{C\mu}{1 - (S-1)\mu} \qquad (38)$$

AND

$$u_s = \frac{C(1+\mu)}{1 - (S-1)\mu} \qquad (39)$$

$$P_H = \rho_0 u_s u_p = \frac{\rho_0 C^2 \mu(\mu+1)}{[1 - (S-1)\mu]^2} \qquad (40)$$

SIMILARLY

$$E_H = \frac{P_H V_0}{2} \frac{\mu}{\mu+1} \qquad (42)$$

SUBSTITUTING EQS (40) AND (42) INTO (34)

$$P = \frac{\rho_0 C^2 \mu(\mu+1)(1 - \frac{\gamma\mu}{2})}{[1 - (S-1)\mu]^2} + \frac{\gamma}{V} E \qquad (43)$$

γ CAN BE OBTAINED, FOR EXAMPLE, FROM HUGONIOT AND DOUBLE-SHOCK DATA AT THE SAME VOLUMES.

THIS EQUATION OF STATE CAN BE USED IN FINITE-DIFFERENCE COMPUTER SIMULATIONS TO DESIGN SHOCK-WAVE EXPERIMENTS OR TO INTERPRET THEM.

MCQUEEN ET AL (1970) SHOWED THAT A GOOD APROXIMATION IS $\frac{\gamma}{V} = \text{CONSTANT} = \frac{\gamma_0}{V_0}$

THE GRUNEISEN EQUATION OF STATE IS USEFUL FOR SIMULATING SHOCK-WAVE EXPERIMENTS. FOR A PURE FLUID THE SYSTEM OF EQUATIONS IS:

$$\rho \frac{\partial u}{\partial t} = -\frac{\partial (P+Q)}{\partial x} \qquad \text{EQ. OF MOTION}$$

$$\frac{\partial V}{\partial t} = V \frac{\partial u}{\partial x} \qquad \text{EQ. OF CONTINUITY}$$

$$\frac{\partial E}{\partial t} = -(P+Q) \frac{\partial V}{\partial t} \qquad \text{ENERGY EQ.}$$

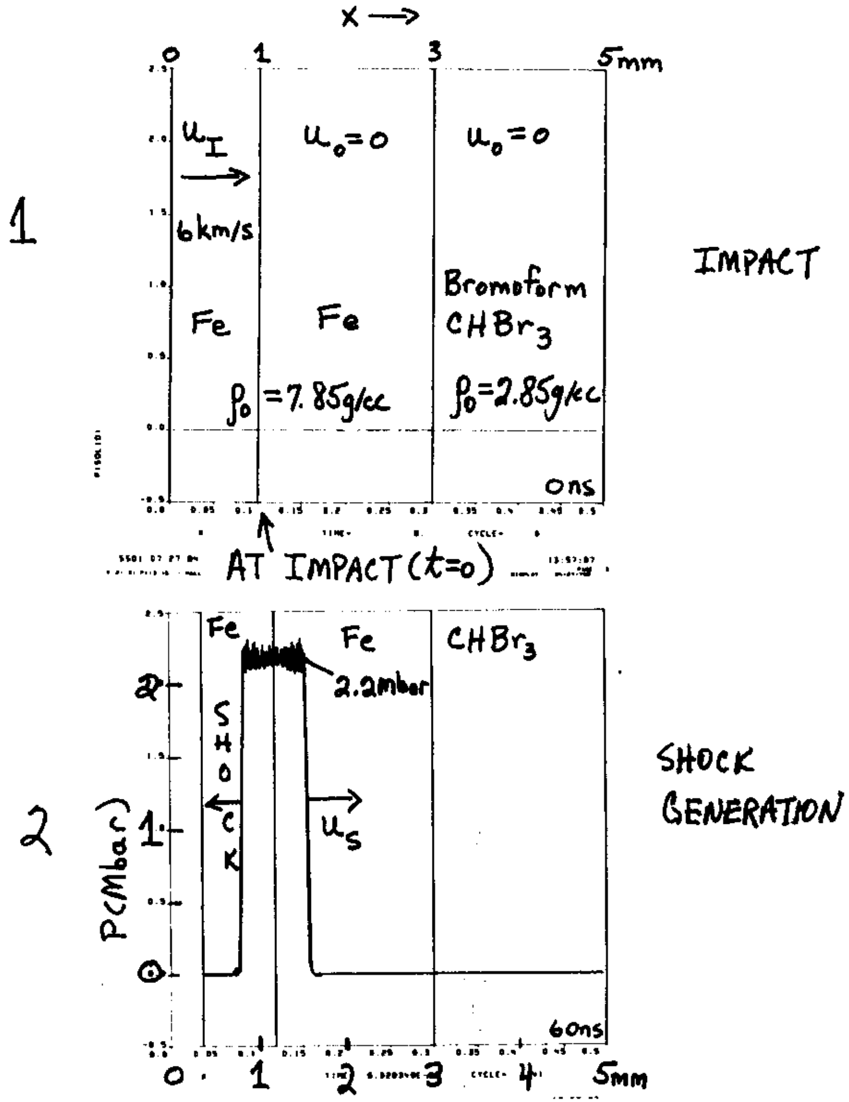
Q = ARTIFICIAL VISCOSITY — NUMERICAL WAY TO TRACK SHOCK DISCONTINUITIES

$$V \rightarrow V + \Delta V$$
$$E \rightarrow E + \Delta E$$
$$P(V,E) \rightarrow P(V+\Delta V,\ E+\Delta E)$$

SOLVED BY FINITE-DIFFERENCE NUMERICAL INTEGRATION

GRUNEISEN EOS

WE WILL NOW SHOW A WAVE CALCULATION FOR THE CASE OF AN Fe IMPACTOR STRIKING AN Fe TARGET FOLLOWED BY SHOCK TRANSMISSION INTO A DENSE FLUID:



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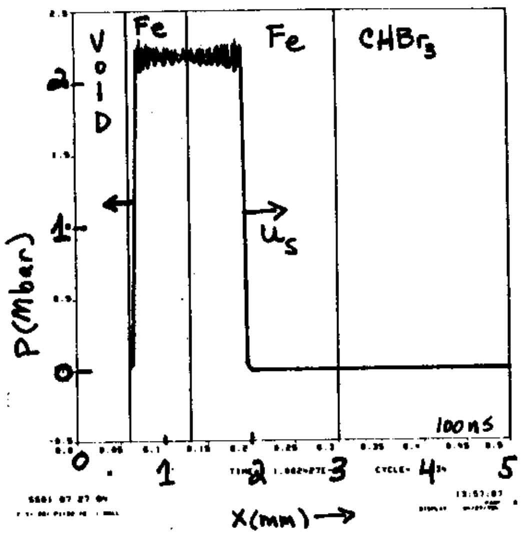
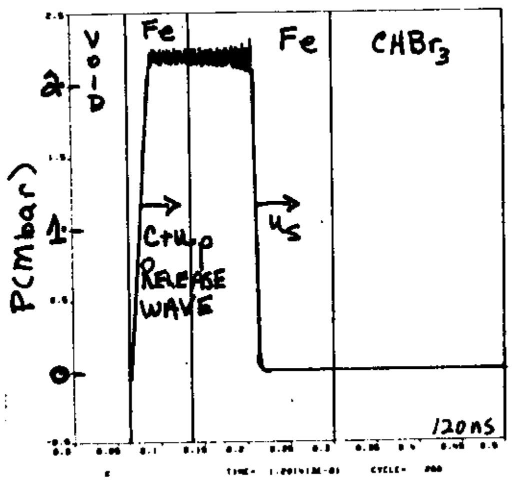


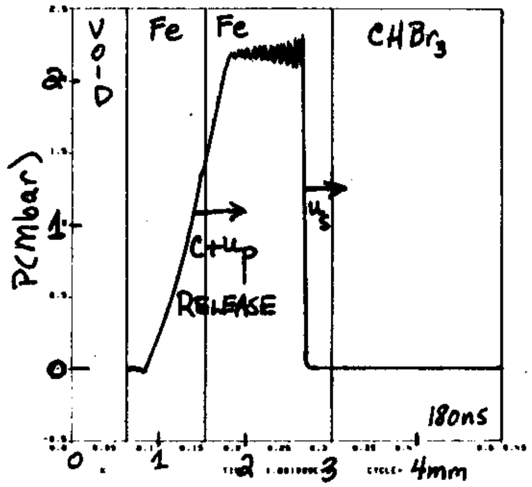
SHOCK ABOUT TO REACH REAR OF Fe IMPACTOR

4



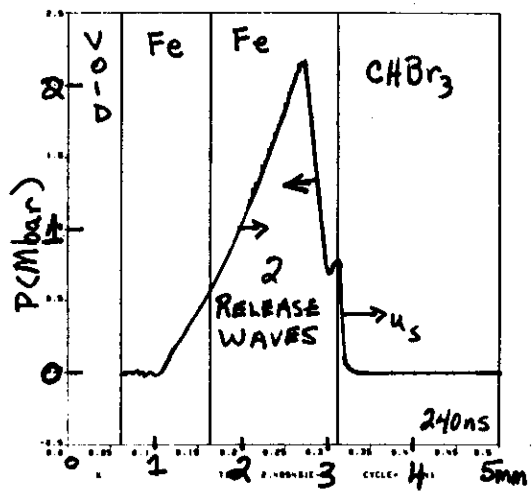
PRESSURE RELEASE WAVE FROM REAR SURFACE IS GENERATED

5



SHOCK IN Fe APPROACHES LIQUID

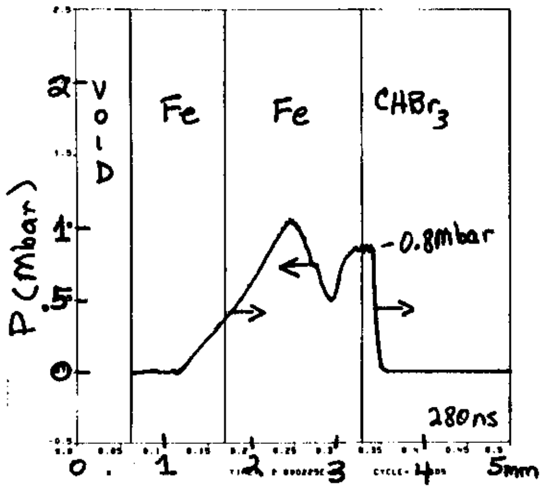
6



SHOCK IS TRANSMITTED INTO $CHBr_3$

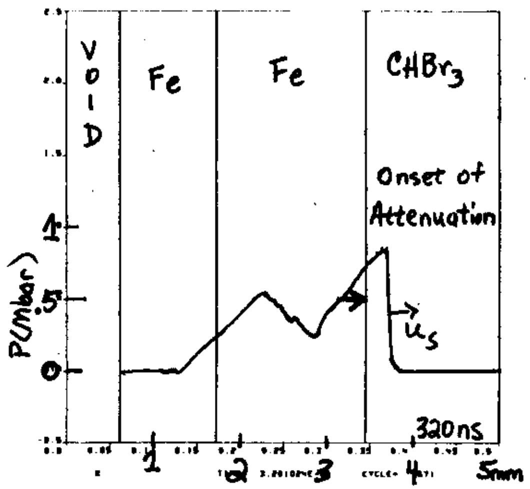
RELEASE WAVE IS REFLECTED BACK INTO Fe

7



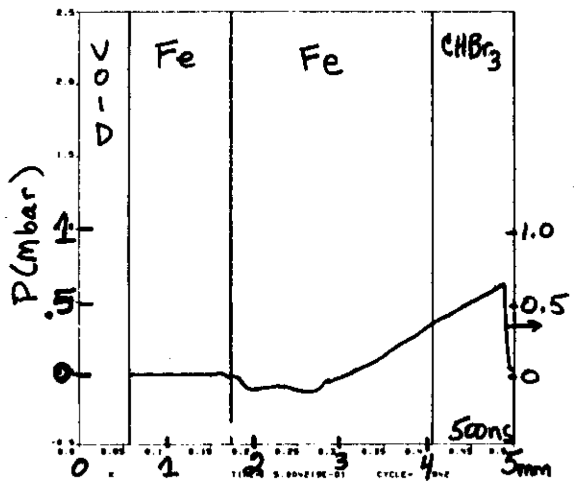
SHOCK IN $CHBr_3$

8



SHOCK IN $CHBr_3$ STARTS TO ATTENUATE

9



SIMPLE ATTENUATING SHOCK

THIS CALCULATION IS A SIMULATION OF THE BROWN AND MCQUEEN EXPERIMENT TO MEASURE LONGITUDINAL SOUND VELOCITIES.

FOR THIS CALCULATION THE FOLLOWING GRUNEISEN EQUATIONS OF STATE WERE USED:

	C (cm/μs)	S	γ	ρ_0 (g/cc)
Fe	0.357	1.92	1.2	7.85
$CHBr_3$	0.18	1.2	0.5	2.85

SHOCK TEMPERATURE

SHOCK TEMPERATURES OF OPTICALLY TRANSPARENT MATERIALS HAVE BEEN MEASURED. THE METHOD ASSUMES THAT THE SHOCK FRONT IS OPTICALLY THIN (WEAK OPTICAL LIGHT ABSORBER) AND THAT THERMAL RADIATION EMITTED FROM THE SHOCK FRONT IS REPRESENTATIVE OF MATERIAL IN THERMAL EQUILIBRIUM BEHIND THE SHOCK FRONT.

FOR EXAMPLE, WATER MEASUREMENTS WERE PERFORMED AT THE LAWRENCE LIVERMORE NATIONAL LABORATORY (LLNL) TWO-STAGE GUN BY LYZENGA *et al.*, 1982. THE SPECIMEN HOLDER:

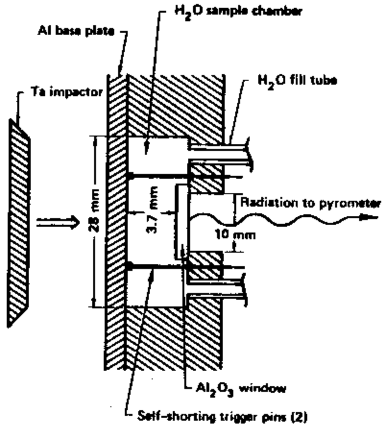


FIG. 15. Illustration of target containing transparent liquid, e.g. water, for pyrometric temperature measurement experiments by Lyzenga *et al.*[42]

THE IMPACTOR STRIKES THE AL BASEPLATE AND GENERATES A HIGH SHOCK PRESSURE (500-800 KBAR). THE SHOCK IS TRANSMITTED THROUGH THE ALUMINUM AND INTO THE LIQUID. THE SHOCK-COMPRESSED WATER BEHIND THE SHOCK FRONT IS HEATED TO 3000-5000 K, BECOMES OPAQUE, AND EMITS THERMAL RADIATION. THE RADIATION IS TRANSMITTED THROUGH THE AS-YET UNCOMPRESSED, TRANSPARENT LIQUID, THROUGH THE SAPPHIRE WINDOW, TO A TURNING MIRROR WHICH REFLECTS THE RADIATION TO A 6-CHANNEL PYROMETER

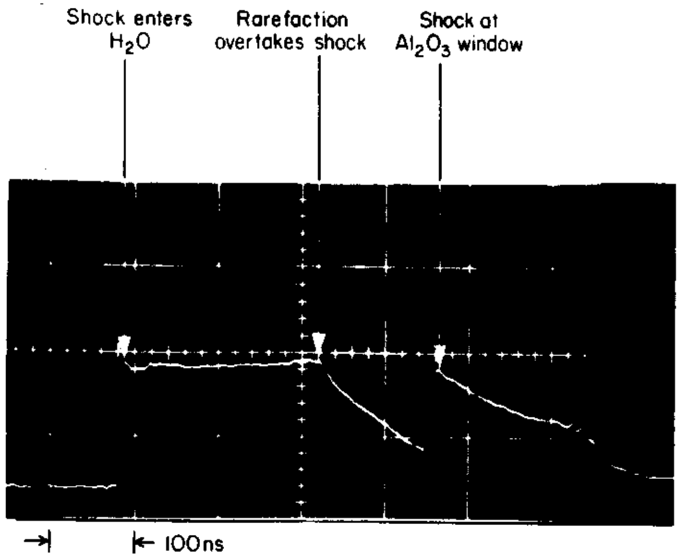


FIG. 3. Experimental record from a shock decaying from 59 GPa on shot WET5. A rarefaction overtakes and attenuates the shock wave at the indicated time. Each horizontal division is 100 ns.

USING NARROW-BAND, FILTERED, OPTICAL DIODES AS DETECTORS. AN OSCILLOGRAM FROM ONE DIODE FROM AN EXPERIMENT WHICH ACHIEVED 585 KBAR AND 3830 K IS SHOWN ON THE PREVIOUS PAGE. THE VOLTAGE SIGNAL RISES RAPIDLY AS THE SHOCK ENTERS THE WATER, REMAINS STEADY UNTIL THE RELEASE WAVE FROM THE REAR OF A THIN Cu IMPACTOR OVERTAKES THE SHOCK — AT WHICH POINT SHOCK PRESSURE, TEMPERATURE, AND OPTICAL EMISSION DECREASE. THE SIGNAL RISES AGAIN WHEN THE SHOCK STRIKES THE Al_2O_3 WINDOW AND THE WATER IS DOUBLE-SHOCKED TO HIGHER PRESSURE AND TEMPERATURE. THE DATA FIT A BLACK BODY SPECTRUM. THE FITS TO THE INTENSITY DATA ARE SHOWN ON THE NEXT PAGE. ALSO SHOWN IS A PLOT OF SHOCK TEMPERATURE VERSUS PRESSURE. THESE DATA ARE CONSISTENT WITH A CONSTANT HEAT CAPACITY OF $C_V = 8.7\ R/mol\ H_2O$, WHICH IS VERY CLOSE TO THE VALUE OF 1 CAL/G AT AMBIENT.

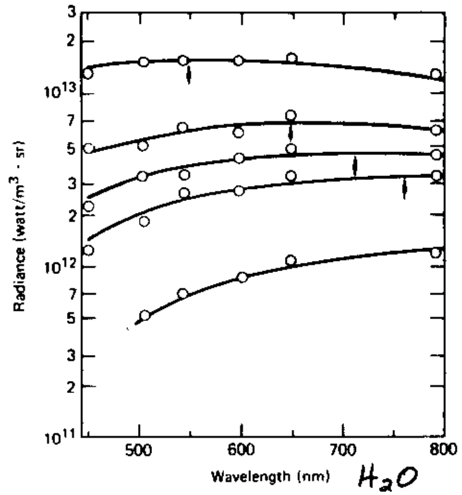


FIG. 4. Spectral radiance for all experiments. Circles are data. Solid curves are best fits using temperatures and emissivities listed in Table I. Arrows point to maxima in fitted spectra.

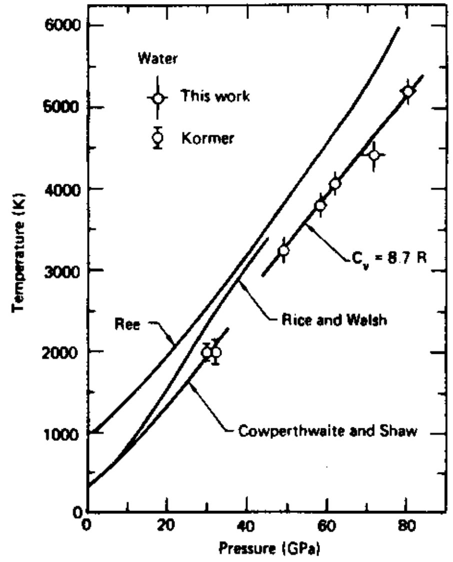


FIG. 5. H_2O shock temperature data plotted as a function of pressure. Results of the current investigation are shown with those of Kormer (Ref. 1). The line through high-pressure data was calculated by the method described in the text. Theoretical calculations are from Refs. 3, 5, and 7.

THIS TECHNIQUE WAS ALSO APPLIED TO FUSED AND α-QUARTZ. DATA OBTAINED BY AHRENS et al, 1982 AT THE LLNL TWO-STAGE GUN IS SHOWN ON THE NEXT PAGE. THE STRUCTURE IN THE T-P DATA IS PROBABLY CAUSED BY MELTING OF STISHOVITE. THE CHARACTERISTICS OF THE MELT TRANSITION AT 700 KBAR ARE:

MELT TEMPERATURE, T_m,	4400 K (±5%)
SLOPE dT_m/dP	1 K/KBAR (±50%)
VOLUME CHANGE $\Delta V/V$	~4%
LATENT HEAT OF FUSION	3.5 MJ/KG (±15%)

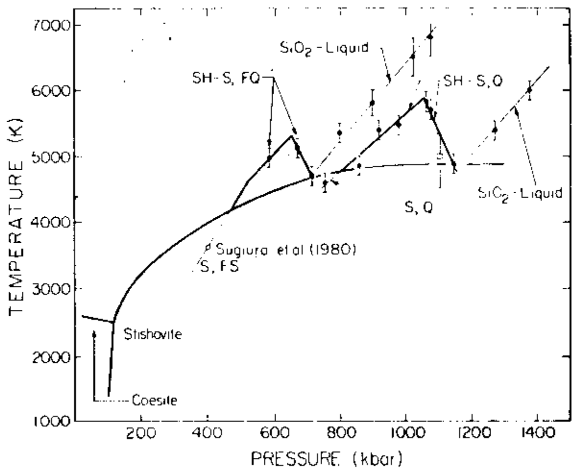
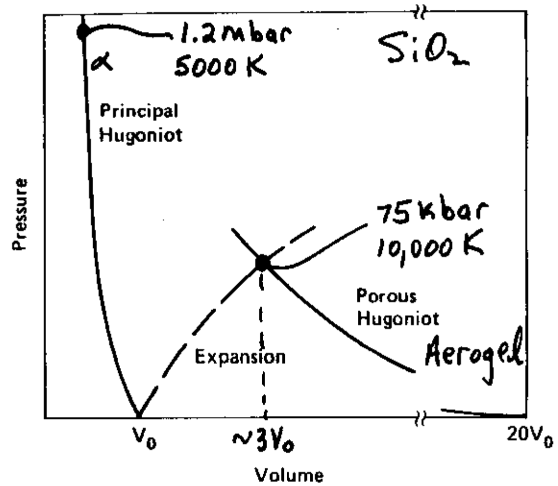


Fig. 8. SiO_2 Hugoniot temperatures and pressures and the SiO_2 phase diagram. Proposed phase boundary between stishovite and liquid phase is drawn through temperature minima, assuming that super-heating of the solid occurs in the shock wave. The coesite-stishovite-liquid triple point is estimated from JACKSON (1976). Heavy lines indicate regions where we believe stishovite is super-heated above melting point. S, FS indicates stishovite from fused quartz; SH-S, FQ indicates super-heated stishovite from fused quartz; S, Q indicates stishovite from quartz; and SH-S, Q indicates super-heated stishovite from quartz. Square symbol datum from Boslough and Ahrens (unpublished).

THE ABOVE FIGURE INDICATES THAT TEMPERATURES ALONG THE FUSED QUARTZ (ρ_0=2.2g/cc) HUGONIOT ARE HOTTER THAN FOR α-QUARTZ (ρ_0=2.65g/cc). IN GENERAL SHOCKING A MATERIAL FROM AN EXPANDED VOLUME PRODUCES MORE THERMAL ENERGY AND HIGHER TEMPERATURES. POROUS MATERIALS HAVE BEEN STUDIED EXTENSIVELY FOR THIS REASON.

RECENTLY VERY UNIFORM, TRANSPARENT, ULTRA-FINE-GRAINED (~100 Å pore size), 20-FOLD EXPANDED (ρ_0=0.13 g/cc) SiO_2 HAS BEEN SHOCK-COMPRESSED (HOLMES, et al, 1984). FINAL DENSITIES WERE 3-FOLD EXPANDED RELATIVE TO α-QUARTZ AT PRESSURES OF 150 KBAR AND MEASURED TEMPERATURE OF 10,000 K. THUS, HOT, EXPANDED SiO_2 HAS BEEN STUDIED BY SHOCK COMPRESSION. THE RESULTS ARE ILLUSTRATED:



THE EQUATION OF STATE OF HOT EXPANDED STATES IS RELEVANT TO VOLCANISM (MAGMA) AND METEORITE-INDUCED CRATERING.

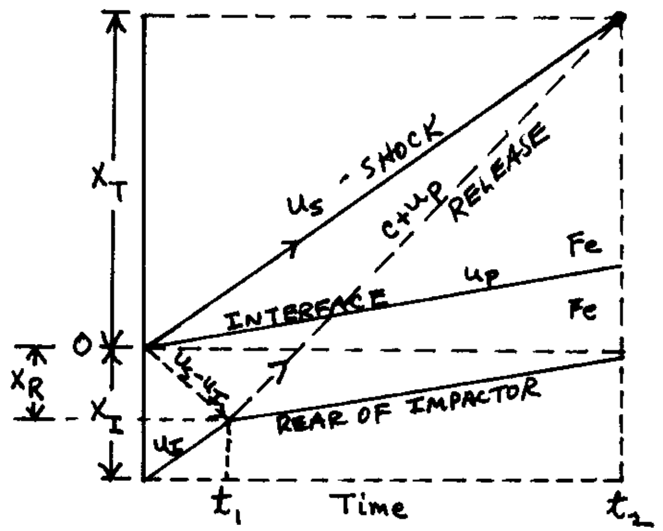
SOUND VELOCITY MEASUREMENTS

MEASUREMENT OF RELEASE WAVE (SOUND) VELOCITY IN SHOCKED SOLIDS IS A USEFUL TECHNIQUE TO DETECT PHASE TRANSITIONS AT ULTRA-HIGH PRESSURES. THE TECHNIQUE IS BASED ON EQ. (25)

$$C_B^2 = C_L^2 - \frac{4}{3} C_T^2 ,$$

WHERE C_L IS THE LONGITUDINAL SOUND VELOCITY, C_T IS THE TRANSVERSE (SHEAR) VELOCITY, AND C_B IS THE BULK SOUND VELOCITY. SOUND VELOCITIES ARE EXPECTED TO BE A MORE SENSITIVE INDICATION OF PHASE CHANGES THAN P-V BECAUSE SOUND VELOCITIES ARE RELATED TO DERIVATIVES OF P-V.

PHASE TRANSITIONS IN Fe HAVE BEEN OBSERVED AT ~2 MBAR (BROWN AND McQUEEN, 1982). THE EXPERIMENT CONSISTS IN MEASURING THE EXACT POSITION AT WHICH THE LONGITUDINAL RELEASE VELOCITY OVERTAKES THE SHOCK. THE RELATION IS DERIVED AS FOLLOWS.



X_I = IMPACTOR THICKNESS

X_T = TARGET THICKNESS AT WHICH RELEASE FROM REAR OF IMPACTOR OVERTAKES SHOCK

t_1 = TIME IMPACT SHOCK REACHES REAR OF IMPACTOR

t_2 = TIME OF OVERTAKE

$$X_I = u_I t_1 + (u_s - u_I) t_1 = u_s t_1 \Rightarrow t_1 = \frac{X_I}{u_s} \qquad (44)$$

$$X_T = u_s t_2 \Rightarrow t_2 = \frac{X_T}{u_s} \qquad (45)$$

$$X_T + X_R = (c + u_p)(t_2 - t_1) \qquad (46)$$

$$X_R = (u_s - u_I) t_1 \qquad (47)$$

$$\frac{c}{u_s}\left(1 - \frac{t_1}{t_2}\right) = \left(1 - \frac{u_p}{u_s}\right)\left(1 + \frac{t_1}{t_2}\right) \qquad (48)$$

$$\frac{t_1}{t_2} = \frac{X_I}{X_T} \equiv \frac{1}{R} \qquad (49)$$

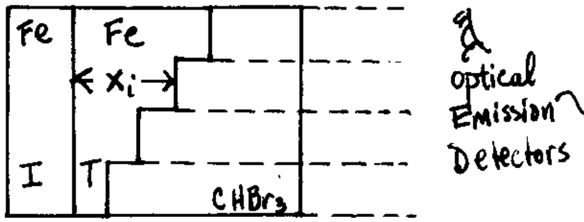
52

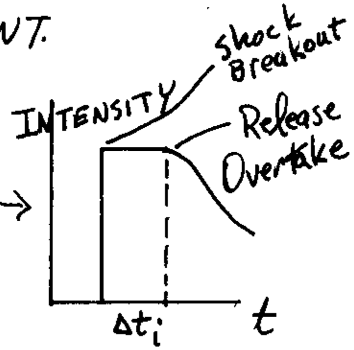
$$1-\frac{u_p}{u_s} = \frac{V}{V_0} = \frac{\rho_0}{\rho} \qquad (2)$$

$$\boxed{C = u_s\left(\frac{\rho_0}{\rho}\right)\left(\frac{R+1}{R-1}\right)} \qquad (50)$$

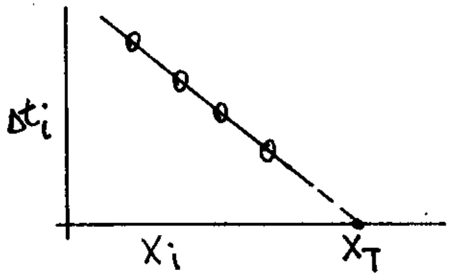
IN AN IMPACT EXPERIMENT u_I IS MEASURED. ρ AND u_s ARE OBTAINED BY SHOCK IMPEDANCE MATCHING. ρ_0 AND X_I ARE MEASURED PRIOR TO THE EXPERIMET.

X_T IS OBTAINED BY MEASURING TIME-RESOLVED OPTICAL BRIGHTNESS — SIMILAR TO A SHOCK TEMPERATURE MEASUREMENT.





Plot $(x_i, \Delta t_i)$:



53

Fe RESULTS OF BROWN AND MCQUEEN (1980):

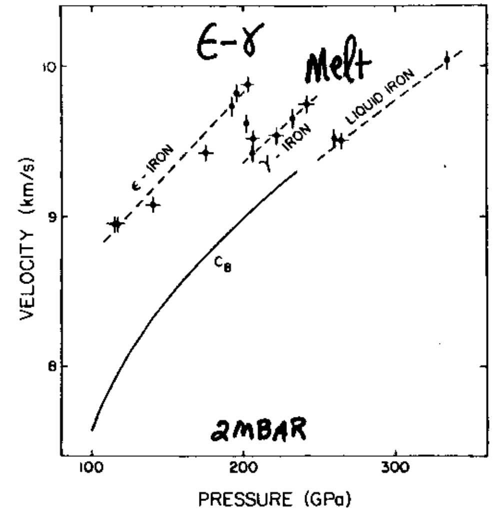
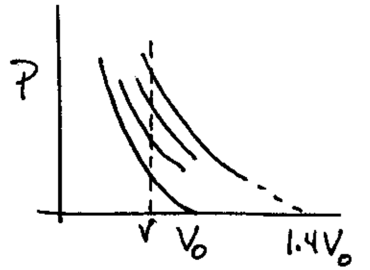


Fig. 1. Elastic wave velocities as a function of pressure along the Hugoniot of iron. The solid curve is the calculated bulk sound velocity (from BROWN and MCQUEEN, 1980, 1982).

THE DISCONTINUITIES AT 2.0 AND 2.5 MBAR ARE INTERPRETED AS PHASE CHANGES. THE AGREEMENT BETWEEN THE DATA AND THE CALCULATED BULK SOUND VELOCITY SUGGEST THAT THE 2.5 MBAR TRANSITION IS MELTING. THE LOWER PRESSURE ONE IS THEN ASCRIBED TO THE ε-γ PHASE TRANSITION.

NOTE THAT THE U_s-U_p DATA FOR Fe SHOWED NO INDICATIONS OF PHASE TRANSITIONS.

BROWN AND MCQUEEN MEASURED THE GRUNEISEN PARAMETER FOR Fe BY PERFORMING HUGONIOT EXPERIMENTS ON POROUS Fe. THEY FOUND $(\partial P/\partial E)_V = 0.06 \pm 0.01\ m^3/Mg$ AND $\gamma = V(\partial P/\partial E)_V$. THEY CALCULATED THE TEMPERATURE OF THE HUGONIOT, $\epsilon - \gamma$ PHASE TRANSITION, MELT LINE TAKING INTO ACCOUNT



LATTICE AND ELECTRONIC CONTRIBUTIONS TO THE HEAT CAPACITY AND ESTIMATING THE LATENT HEAT OF THE PHASE TRANSITIONS. TAKING INTO ACCOUNT ESTIMATED UNCERTAINTIES IN THE CALCULATION THEY PROPOSE:

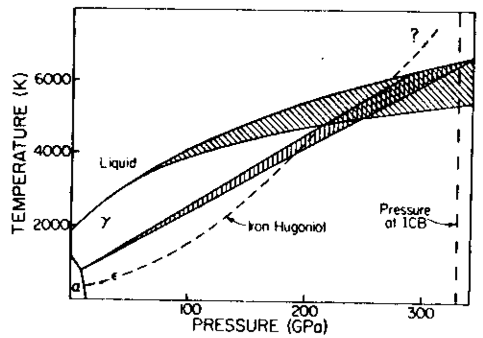
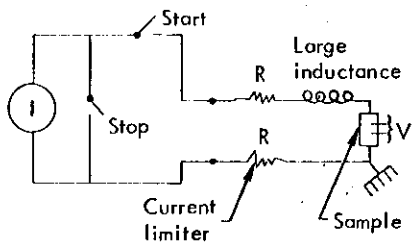


Fig. 2. Phase diagram for pure iron which is consistent with the shock-wave data. Bounds shown for the phase boundaries reflect uncertainties in temperatures along the Hugoniot of iron.

UNCERTAINTIES IN TEMPERATURE ARE 500-1000 K AT 5000 K. THUS, WORK IS STILL NEED TO PIN DOWN THE TEMPERATURE OF THE CORE.

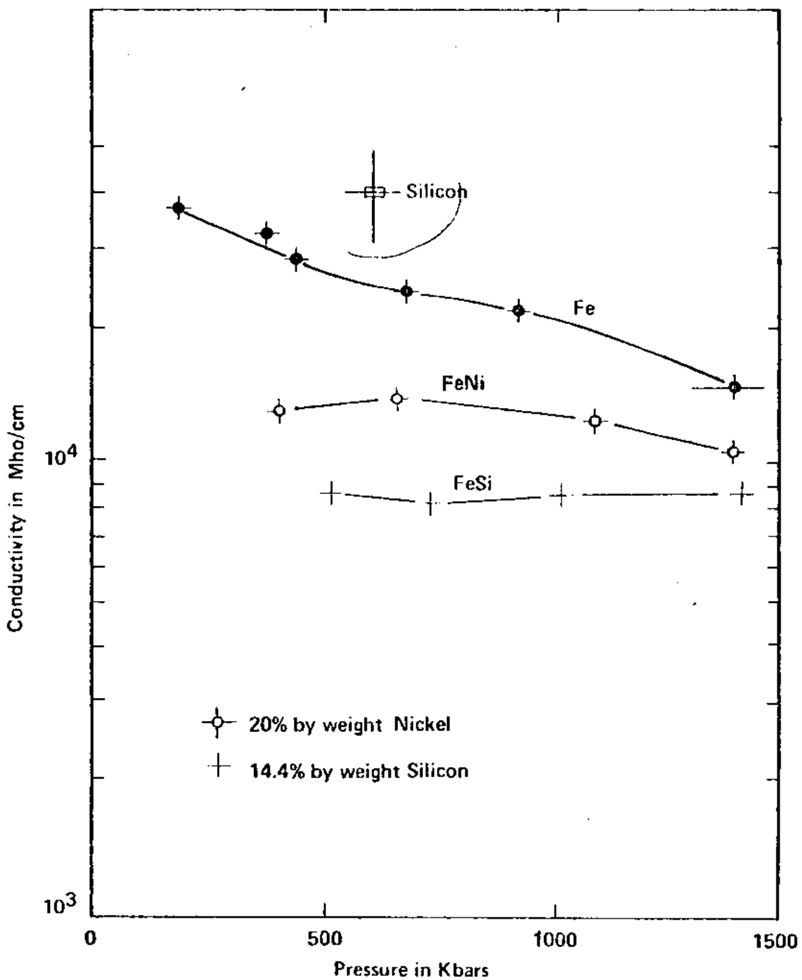
ELECTRICAL CONDUCTIVITY

ELECTRICAL CONDUCTIVITY OF Fe AND FeNi AND FeSi ALLOYS WAS MEASURED BY MATASSOV (1977). HE USED A 4-PROBE TECHNIQUE AND SANDWICHED THE SPECIMEN IN AN Al_2O_3 HOLDER. LARGE CURRENT WAS PULSED THROUGH THE SAMPLE AND THE VOLTAGE ACROSS THE SAMPLE WAS MONITORED ON AN OSCILLOSCOPE. THE CIRCUIT IS ILLUSTRATED



Constant current circuit

MATASSOV'S DATA TO 1.4 MBAR IS SHOWN:



THE SPECIMEN HOLDER FOR LIQUIDS AND CIRCUIT FOR CONDUCTIVITY MEASUREMENTS ARE SHOWN FROM MITCHELL AND NELLIS (1982):

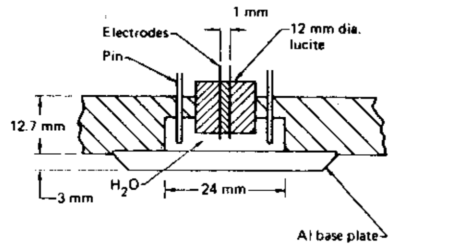


FIG. 3. Water specimen holder for electrical conductivity measurements using the two-stage gun. Impactor is incident from below.

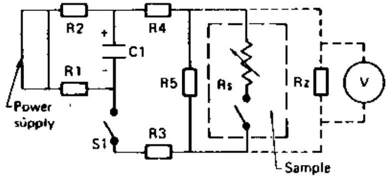


FIG. 4. Electrical conductivity measuring circuit.

THIS IS A TWO-PROBE TECHNIQUE. THE SPECIMEN IS INITIALLY AN INSULATOR AND CURRENT FLOWS ONLY THROUGH THE SHUNT RESISTANCE R_5. WHEN THE SPECIMEN IS SHOCKED AND CONDUCTS, CURRENT FLOWS THROUGH R_s AS WELL. THE VOLTAGE DROP ACROSS THE PARALLEL COMBINATION OF R_5 AND R_s IS MEASURED ON AN OSCILLOSCOPE. CONDUCTIVITY IS DERIVED FROM CELL RESISTANCE BY INDEPENDENT CALIBRATION.

THE DATA FOR SHOCKED WATER IS SHOWN BELOW. THE HIGH CONDUCTIVITY OF 30 (OHM-CM)$^{-1}$ IS INTERPRETED IN TERMS OF SIGNIFICANT MOLECULAR IONIZATION:

$2H_2O \rightarrow OH^- + H_3O^+$.

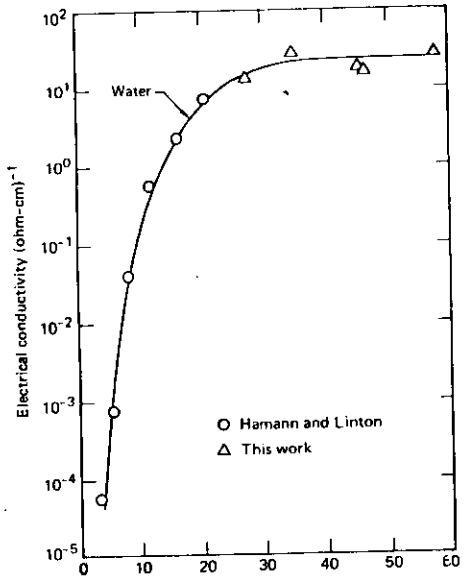


FIG. 10. Electrical conductivity vs shock pressure for liquid H_2O (10 GPA = 100 kbar).

FLASH X-RAY DIFFRACTION

FLASH X-RAY DIFFRACTION PROBES SHOCK-COMPRESSED SOLIDS ON AN ATOMIC SCALE. THIS TECHNIQUE HAS DEMONSTRATED THAT LONG-RANGE ATOMIC ORDER CAN EXIST IN STRONGLY SHOCKED CRYSTALS BELOW MELT AND THAT THE VOLUME COMPRESSION DEDUCED FROM THE MEASURED DECREASE IN LATTICE PARAMETER AGREES WITH THE COMPRESSION CALCULATED FROM THE RANKINE-HUGONIOT RELATIONS (JOHNSON AND MITCHELL, 1980). LiF WAS STUDIED TO 110 GPA (1.1 MBAR). THE EXPERIMENT IS ILLUSTRATED:

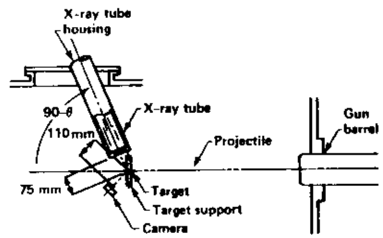


FIG. 14. Illustration of flash X-ray diffraction experiment of Johnson et al.[40] (Reproduced by kind permission of the American Institute of Physics.)

AN INTENSE, 80-ns X-RAY PULSE IS DIRECTED TOWARD THE REAR SURFACE OF THE CRYSTAL JUST BEFORE SHOCK ARRIVAL. A SMALL FILM CASSETTE IS POSITIONED TO DETECT

BRAGG-SCATTERED X-RAYS FOR BOTH THE SHOCKED AND UNSHOCKED STATE. THE COMPRESSION IN UNIT CELL VOLUME DETERMINED FROM THE SHIFT OF THE (200) REFLECTION IS FOUND TO AGREE TO WITHIN 1% WITH HUGONIOT COMPRESSIONS OBTAINED BY SHOCK IMPEDANCE MATCHING. THE RESULT HOLDS FOR CRYSTALS ORIENTED ALONG [100] or [111] USING EITHER Cu OR Mo RADIATION. THE FACT THAT DIFFRACTION OCCURS IN THE SHOCKED SOLID MEANS THAT LONG-RANGE ATOMIC ORDER DOES IN FACT EXIST, AT LEAST IN LiF UP TO 1.1 MBAR SHOCK PRESSURE. THE RECORD FROM A 550 KBAR EXPERIMENT IS SHOWN ON THE NEXT PAGE:

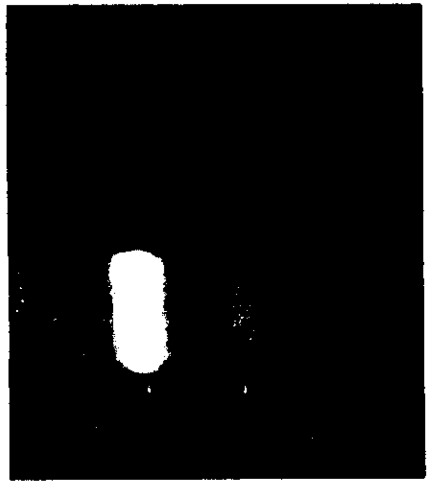


Fig. 8. Flash x-ray diffraction lines from the (200) reflection from single-crystal lithium fluoride using 8-keV copper radiation. The bright diffraction line comes from the unshocked crystal. The lighter line is due to the crystal shocked to 55 GPa. The line shift is a function of the compression of the crystal. The exposure time of the shifted line is about 20 ns. The shifted line is longer than the initial line because the portion of the film above the initial line is masked during the calibration runs.

SHOCK WAVES IN CONDENSED MATTER - 1983
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RAMAN SPECTROSCOPY OF SHOCKED WATER

N. C. Holmes, A. C. Mitchell, W. J. Nellis, W. B. Graham
University of California, Lawrence Livermore National Laboratory
Livermore, California 94550

G. E. Walrafen
Howard University, Washington, D.C. 20059

Raman scattering has been used extensively to study the vibrational and rotational properties of molecules under a variety of conditions. Here our interest is in the behavior of water molecules shocked to high pressures and temperatures. Behind the shock front the water molecules undergo changes in bonding and the molecules may become ionized.[1] Raman spectroscopy can be used to determine the molecular species behind the shock front. In addition, changes in Raman spectra can yield information regarding inter- and intra-molecular potentials and the temperature behind the shock front.

Raman scattering occurs as a result of the differential polarizability of molecules with respect to the inter-atomic separation. The effect is that light incident upon a molecule can excite molecular vibrations. For incident light at ν_i and a molecular vibrational frequency ν_0, scattered light is observed at $\nu = \nu_i \pm \nu_0$. The process for which photons of frequency $\nu_i - \nu_0$ are emitted is termed Stokes scattering and anti-Stokes scattered photons have frequency $\nu_i + \nu_0$. For weak photon fields the effect is linear in intensity and very weak (cross-sections on the order of 10^{-29} cm^2 are typical) and is called spontaneous Raman scattering. When the incident intensity is large the process is non-linear and stimulated Raman scattering occurs. Stimulated Raman backscattering experiments have been performed recently on shocked benzene.[2] Our interest is in spontaneous scattering. This is an inherently broadband technique which lends itself to study of the OH-stretch band in water which can be up to $\sim$1000 cm^{-1} wide. Also, spontaneous scattering does not significantly effect the vibrational thermal equilibrium, allowing it to be used for the determination of temperature.[3]

In our experiments we have observed the OH-stretch band in H_2O shocked to 7 GPa and a temperature of $\sim$370°C.[4,5] The two-stage light-gas gun at LLNL was used to generate the shock wave in liquid water initially at 25°C and atmospheric pressure. A frequency-doubled Nd:glass laser at 532 nm was used to excite the shocked sample. Stokes radiation emitted at a 90° angle to the exciting laser beam was collected by an f/2 achromatic lens which imaged the sample volume onto the slit of an f/3 flat-field 0.25 m spectrograph. A micro-channel plate image intensifier was installed at the focal plane of the spectrograph to increase the brightness of the spectrum which was recorded on film. A spectrum is shown in Fig. 1. The broad peak above a continuum is

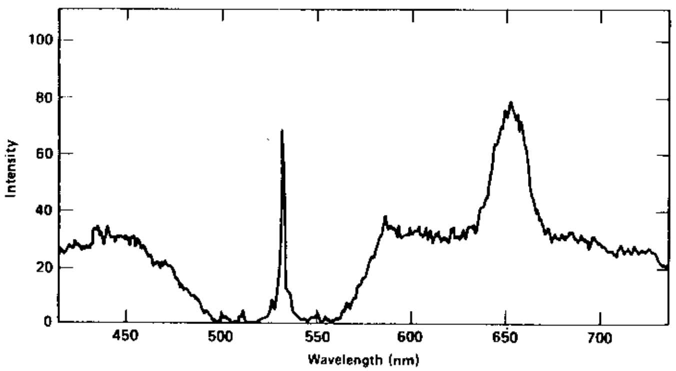


Fig. 1 Spontaneous Raman spectrum of water shocked to 7 GPa.

the observed OH-stretch band in H_2O. The measured width is 690 cm^{-1}. The narrow line is the input laser radiation at 532 nm and the broad continuum, observed in all experiments, is believed to arise from radiation emitted by hot gas compressed on the baseplate of the target by projectile impact. The width of the band is significantly less than that observed in the same sample unshocked (904 cm^{-1}). The narrowing may be due to the breaking of weak hydrogen bonds between water molecules. These bonds are substantially responsible for the very wide OH-stretch band.[6] We also observe a small (+15 cm^{-1}) increase in the Raman shift of shocked H_2O.

The experimental conditions for the spectrum shown were chosen for simplicity. That is, we wished to show feasibility of the technique and chose not to reach conditions of very high temperature and pressures for which anti-Stokes radiation or bands from ionized water molecules are expected. In future experiments we will investigate increasingly high shock pressures to attempt observations of these effects.

We are pleased to acknowledge the technical assistance of C. Wozynski, K. Jeter, G. Governo, W. Thomas, and J. Chmielewski during these experiments.

REFERENCES

1. Hamann, S. D., Properties of Electrolyte Solutions at High Shock Pressures, in Conway, B. E. and Bockris, J. O'M. (eds.) Modern Aspects of Electrochemistry (Plenum, New York, 1974) p. 126-131.

2. Schmidt, S. C., Moore, D. S., Schiferl, D., and Shaner, J. W., Backward Stimulated Raman Scattering in Shock-Compressed Benzene, Phys. Rev. Lett. 50 (1983) 661-664.

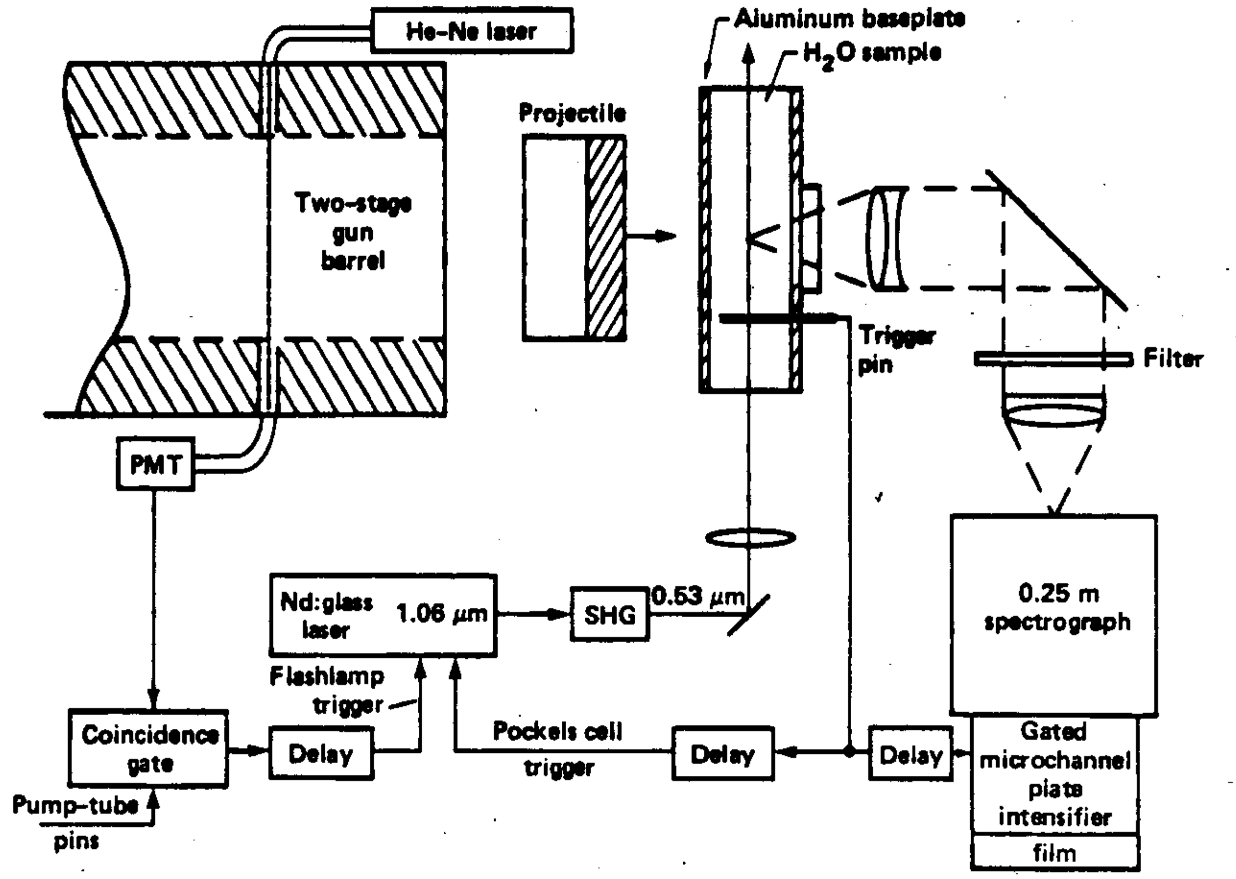
3. Delpuech, A., and Menil, A., Raman Scattering Temperature Measurement behind a Shock Wave, these proceedings.

4. Rice, M. H., and Walsh, J. M., Equation of State of Water to 250 kbars, J. Chem. Phys. 26 (1957) 824-830.

5. Cowperthwaite, M., and Shaw, R., Equation of State for Liquids. Calculation of the Shock Temperature of Carbon Tetrachloride, Nitromethane, and Water in the 100 kbar Region, J. Chem. Phys. 53 (1970) 555-560.

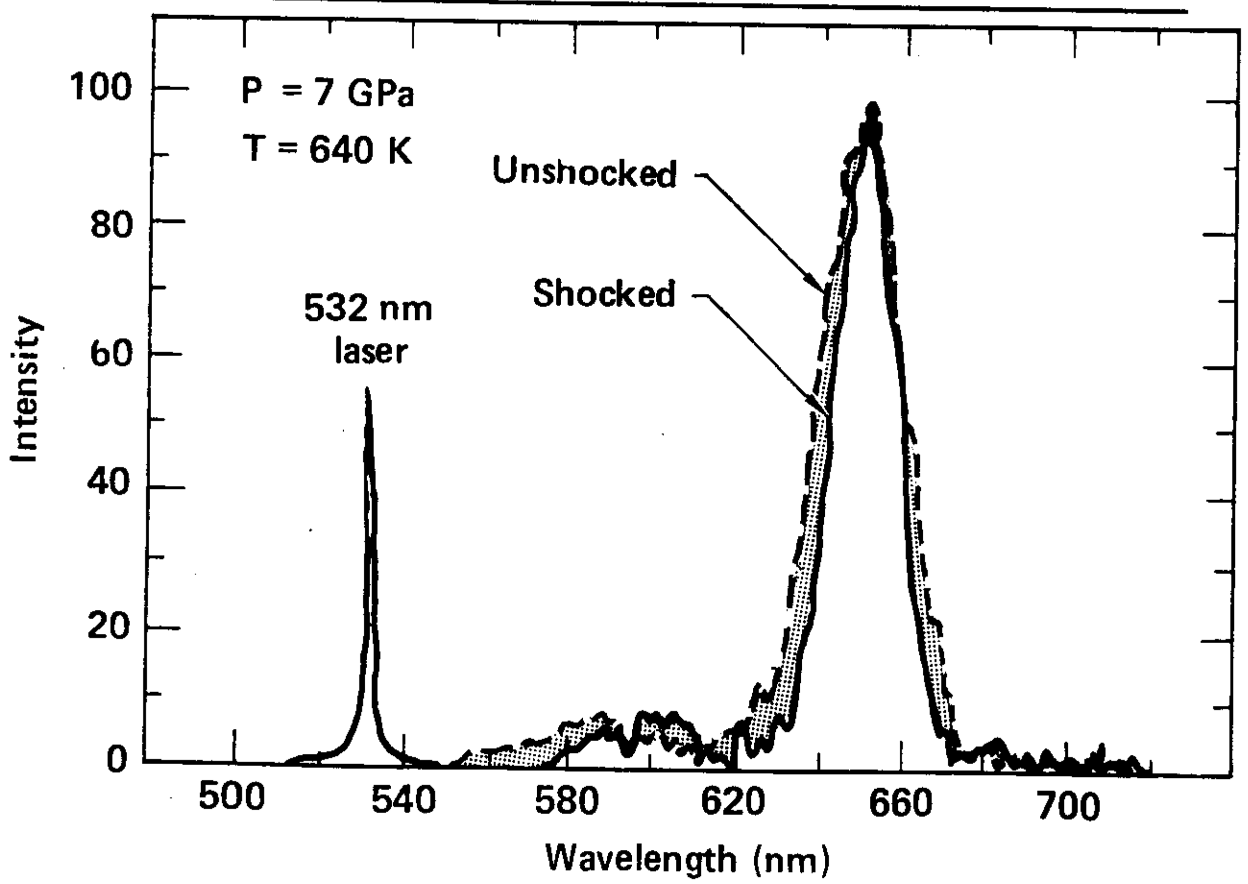
6. Walrafen, G. E., Raman Spectral Studies of the Effects of Temperature on Water Structure, J. Chem. Phys. 47 (1967) 114-126.

SPONTANEOUS RAMAN EXPERIMENT IN SHOCKED WATER



64

Spontaneous raman spectrum of shocked water



65

REFERENCES

AHRENS, T.J., G.A. LYZENGA, AND A.C. MITCHELL, TEMPERATURES INDUCED BY SHOCK WAVES IN MINERALS: APPLICATIONS TO GEOPHYSICS, IN HIGH-PRESSURE RESEARCH IN GEOPHYSICS, EDITED BY S. AKIMOTO AND M.H. MANGHNANI, pp 579-594, CENTER FOR ACADEMIC PUBLICATIONS JAPAN, DORDRECHT, 1982.

BROWN, J.M. AND R.G. MCQUEEN, MELTING IN IRON UNDER CORE CONDITIONS, GEOPHYS. RES. LETT. 7, 533-536, 1980.

BROWN, J.M. AND R.G. MCQUEEN, THE EQUATION OF STATE FOR IRON AND THE EARTH'S CORE, IN HIGH-PRESSURE RESEARCH IN GEOPHYSICS, pp 611-623, 1982.

FRITZ, J.N. AND R.G. MCQUEEN, REFLECTED SHOCKS IN SiO_2, IN SHOCK WAVES IN CONDENSED MATTER-1983, EDITED BY J.R. ASAY, R.A. GRAHAM, AND G.K. STRAUB, ELSEVIER, AMSTERDAM, 1984.

HOLMES, N.C., H.B. RADOUSKY, M.J. MOSS, AND W.J. NELLIS, SILICA AT ULTRAHIGH TEMPERATURE AND EXPANDED VOLUME, TO BE PUBLISHED IN APPL. PHYS. LETT., SEPT, 1984.

HOLMES, N.C., A.C. MITCHELL, W.J. NELLIS, W.B. GRAHAM, AND G.E. WALRAFEN, RAMAN SPECTROSCOPY OF SHOCKED WATER, IN SHOCK WAVES IN CONDENSED MATTER-1983, pp 307-308, 1984.

HOLIAN, B.L. AND G.K. STRAUB, MOLECULAR DYNAMICS OF SHOCK WAVES IN THREE-DIMENSIONAL SOLIDS: TRANSITION FROM NONSTEADY TO STEADY WAVES IN PERFECT CRYSTALS AND IMPLICATIONS FOR THE RANKINE-HUGONIOT CONDITIONS, PHYS. REV. LETT. 43, 1598-1600, 1979.

HOOVER, W.G., STRUCTURE OF A SHOCK-WAVE FRONT IN A LIQUID, PHYS. REV. LETT. 42 1531-1534, 1979.

JOHNSON, Q.J. AND A.C. MITCHELL, FLASH X-RAY DIFFRACTION STUDIES TO 100 GPA, IN HIGH PRESSURE SCIENCE AND TECHNOLOGY, EDITED BY B. VODAR AND P. MARTEAU, pp 977-978, PERGAMON, OXFORD, 1980.

JONES, A.H., W.M. ISBELL, AND C.J. MAIDEN, MEASUREMENT OF THE VERY-HIGH-PRESSURE PROPERTIES OF MATERIALS USING A LIGHT-GAS GUN, J. APPL. PHYS. 37, 3493-3499, 1966.

LYZENGA, G.A., T.J. AHRENS, W.J. NELLIS, AND A.C. MITCHELL, THE TEMPERATURE OF SHOCK-COMPRESSED WATER, J. CHEM. PHYS. 76, 6282-6286, 1982.

MATASSOV, G., THE ELECTRICAL CONDUCTIVITY OF IRON-SILICON ALLOYS AT HIGH PRESSURES AND THE EARTH'S CORE, LAWRENCE LIVERMORE NATIONAL LABORATORY, UCRL-52322, 1977 (UNPUBLISHED Ph.D. THESIS).

MCQUEEN, R.G., J.N. FRITZ, AND S.P. MARSH, ON THE EQUATION OF STATE OF STISHOVITE, J. GEOPHYS. RES. 68, 2319-2322, 1963.

MCQUEEN, R.G., S.P. MARSH, AND J.N. FRITZ, HUGONIOT EQUATION OF STATE OF TWELVE ROCKS, J. GEOPHYS. RES. 72, 4999-5036, 1967.

MCQUEEN, R.G., S.P. MARSH, J.W. TAYLOR, J.N. FRITZ, AND W.J. CARTER, THE EQUATION OF STATE OF SOLIDS FROM SHOCK WAVE STUDIES, IN HIGH-VELOCITY IMPACT PHENOMENA, EDITED BY R. KINSLOW, pp. 293- , ACADEMIC, NEW YORK, 1970.

MITCHELL, A.C. AND W.J. NELLIS, EQUATION OF STATE AND ELECTRICAL CONDUCTIVITY OF WATER AND AMMONIA SHOCKED TO THE 100 GPa (1 MBAR) PRESSURE RANGE, J. CHEM. PHYS. 76, 6273-6281, 1982.

NELLIS, W.J., A.C. MITCHELL, M. VAN THIEL, G.J. DEVINE, R.J. TRAINOR, AND N. BROWN, EQUATION OF STATE DATA FOR MOLECULAR HYDROGEN AND DEUTERIUM AT SHOCK PRESSURES IN THE RANGE 2-76 GPa (20-760 KBAR), J. CHEM. PHYS. 79, 1480-1486.

NELLIS, W.J., MEASUREMENTS AT ULTRA-HIGH DYNAMIC PRESSURE, IN HIGH PRESSURE MEASUREMENT TECHNIQUES, EDITED BY G.N. PEGGS, PP. 69-89, APPLIED SCIENCE, LONDON, 1983.

PAVLOVSKII, A.I., N.P. KOLOKOLCHIKOV, M.I. DOLOTENKO, AND A.I. BYKOV, ISENTROPIC COMPRESSION OF QUARTZ BY THE PRESSURE OF A SUPERSTRONG MAGNETIC FIELD, SOV. PHYS.-JETP LETT. 27, 264-266, 1978.

ROSS, M., R.H. REE, AND D.A. YOUNG, THE EQUATION OF STATE OF MOLECULAR HYDROGEN AT VERY HIGH DENSITY, J. CHEM. PHYS. 79, 1487-1494.

WACKERLE, J., SHOCK-WAVE COMPRESSION OF QUARTZ, J. APPL. PHYS. 33, 922-937, 1962.