

Structures of Solids, Fluids, and Glasses at  
High Pressures and Modest Temperatures

Produced by Dynamic Compression

W. J. Nellis

Harvard University

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## Two examples

Extremely compressible: Hydrogen

Extremely incompressible:  $\text{Gd}_3\text{Ga}_5\text{O}_{12}$  (GGG)

*There are great opportunities for an ERL coupled with dynamic compression because X-ray scattering from dynamically-compressed materials is a virtually unexplored field.*

## What is dynamic compression?

Dynamic compression, as considered here, applies pressures of  $\sim 100$  GPa (1 Mbar) with a rise time to a thermally equilibrated state of  $\sim 1$  ps and a  $\sim 100$  ns duration of that uniform state.

The rise time might be longer for a phase transition.

Pressure causes density to increase.

Because the compression is so fast, the compression is adiabatic and temperature increases.

Shock compression is caused by a single step increase ( $\sim$ ps) in pressure. Quasi-isentropic compression typically occurs over a few 10 ns.

Dynamic compression is tunable over a wide range densities and temperatures within limits.

# Rankine-Hugoniot equations



Relate flow velocities and thermodynamic variables in shocked state to those of initial state

$$P - P_0 = \rho_0 u_s u_p \quad (\text{conservation of momentum})$$

$$V = V_0 [1 - u_p / u_s] \quad (\text{conservation of mass})$$

$$E - E_0 = 1/2 (P + P_0) (V_0 - V) \quad (\text{conservation of energy})$$

**P** is shock pressure

**$u_s$**  is shock velocity

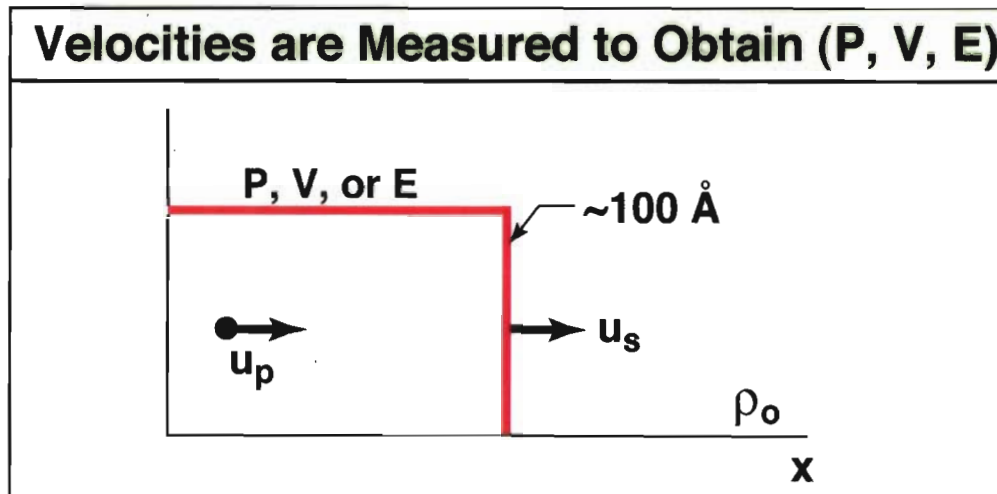
**V** is specific shock volume

**$u_p$**  is mass (particle) velocity

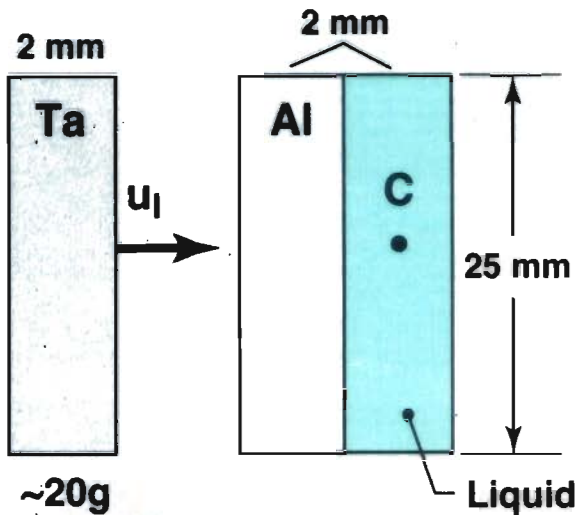
**E** is specific internal shock energy

**$\rho = 1/V$**  is mass density = **D**, density

Zero-subscripted variables refer to the initial state ahead of the shock

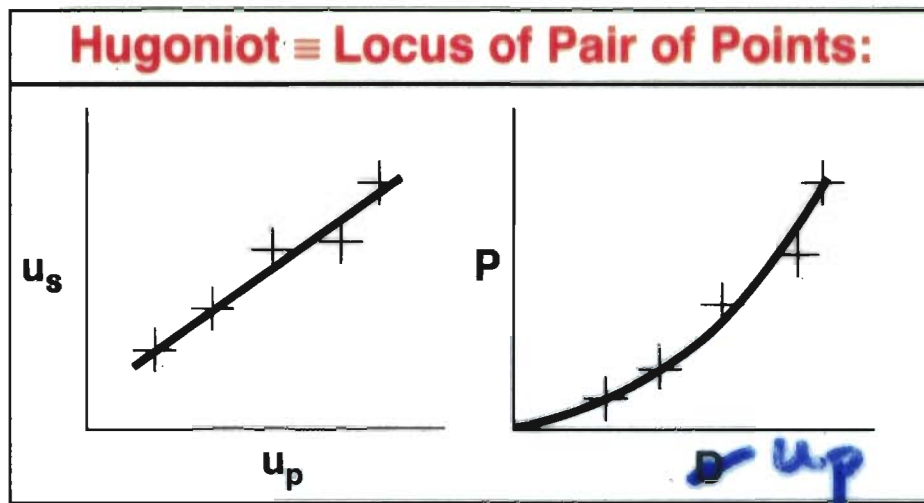
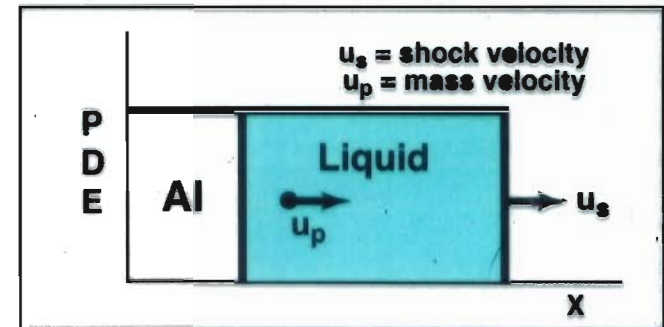
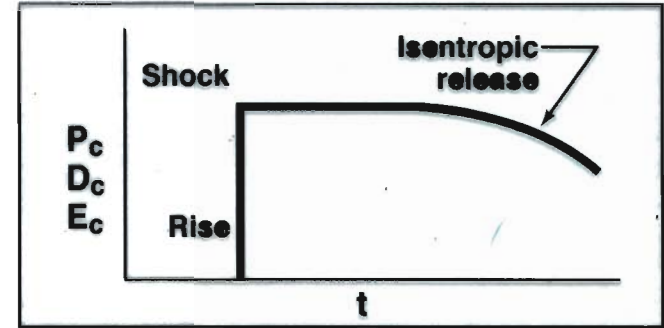


# Single-shock compression of liquid



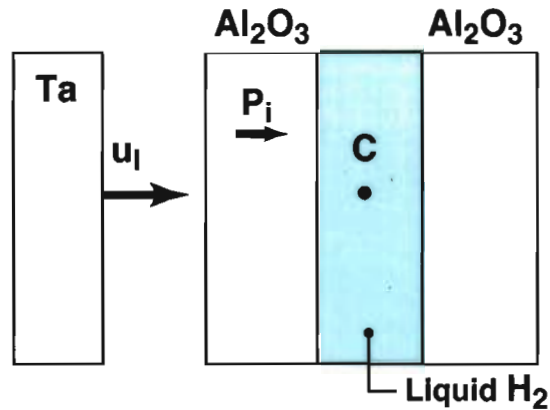
~20g  
~0.5 MJ  
~7 km/s

$P_c$  = Pressure at C  
 $D_c$  = Density at C  
 $E_c$  = Energy at C



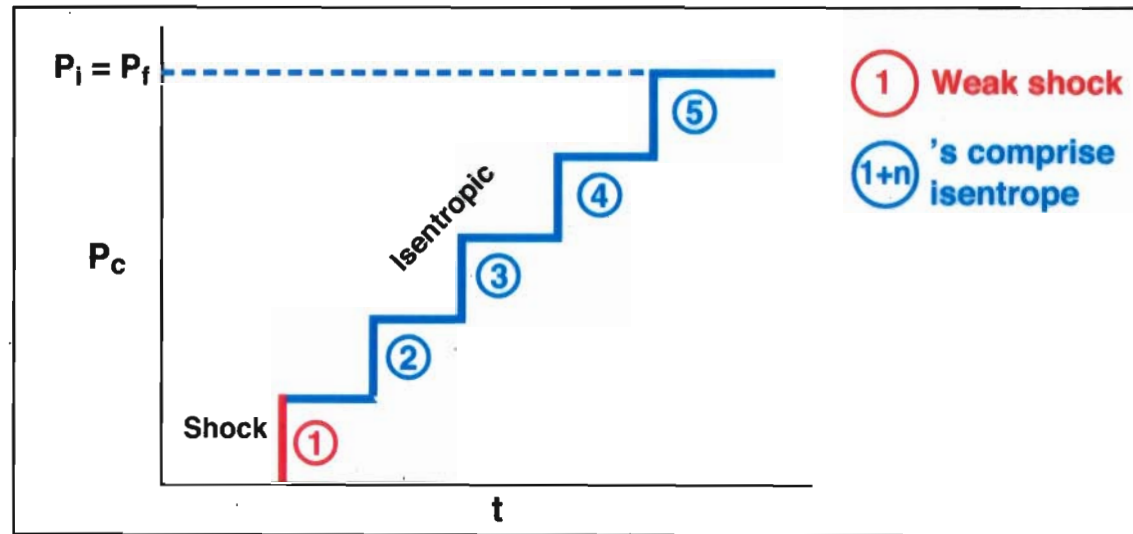
Hugoniot =  
locus of states  
achieved by  
single-shock  
compression

# Reverberating shock compression



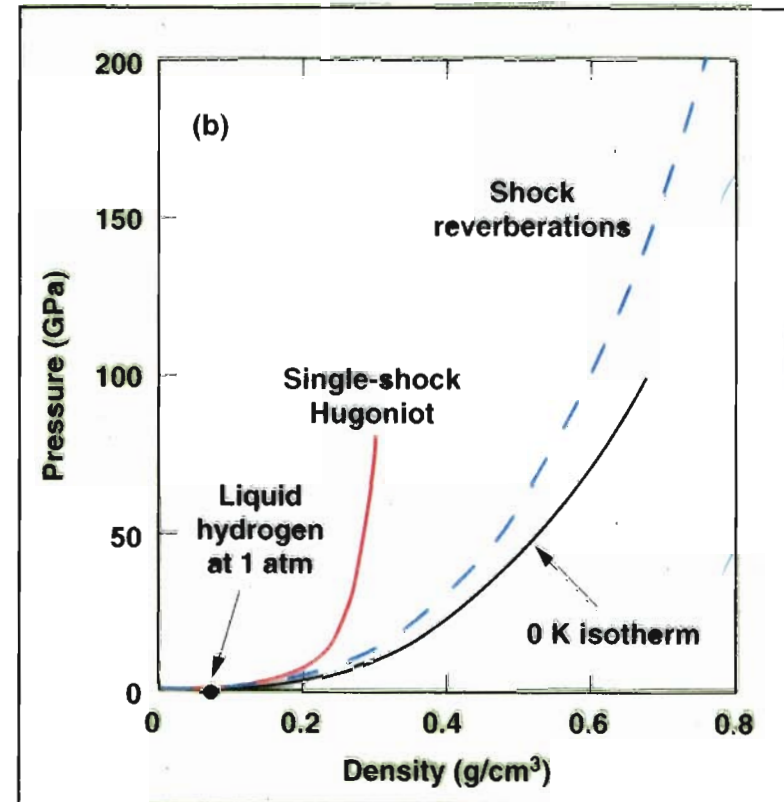
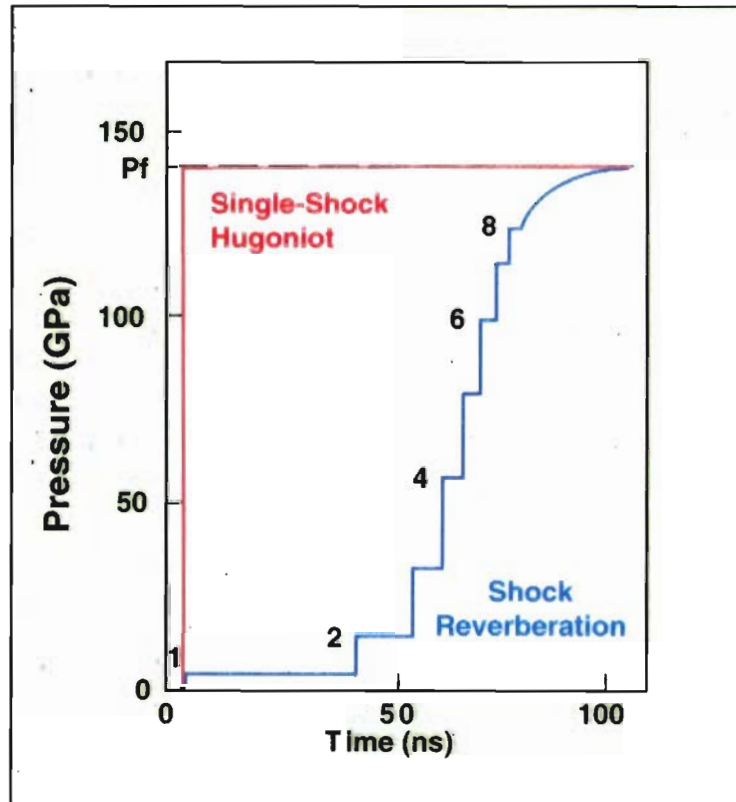
$P_i \equiv$  initial impact shock

$P_f \equiv$  final pressure in hydrogen



Shock reverberation in soft  $H_2$  between stiff sapphire anvils achieves quasi-isentropic compression (weak shock + isentropes)

# Shock Reverberation



shock reverberation states are at **higher density and lower temperatures** than the corresponding **single-shock states**

## Nature of states achieved by dynamic compression

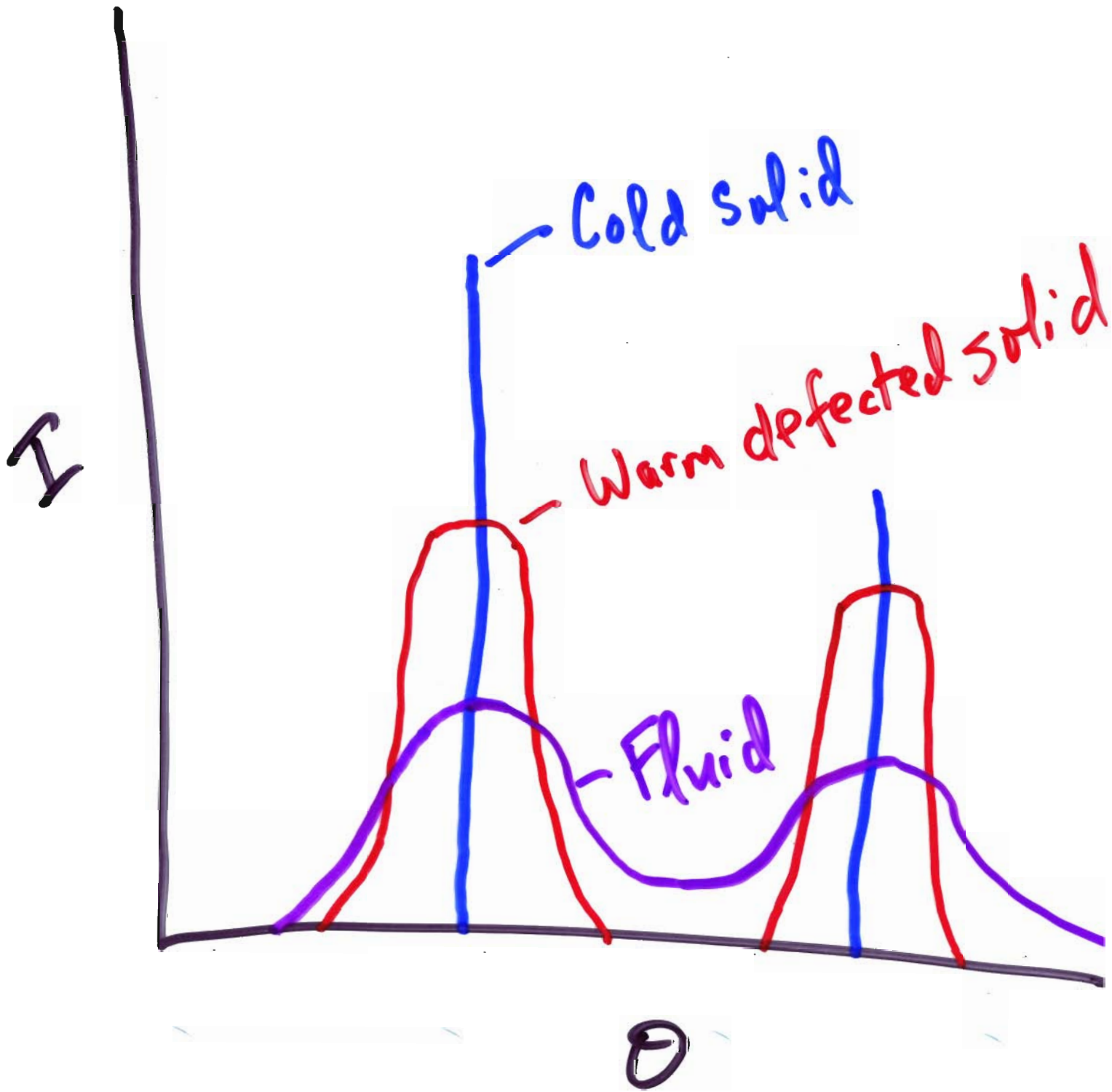
Because temperatures increase,

X-ray diffraction lines of crystallographically ordered solids broaden via the Debye-Waller factor.

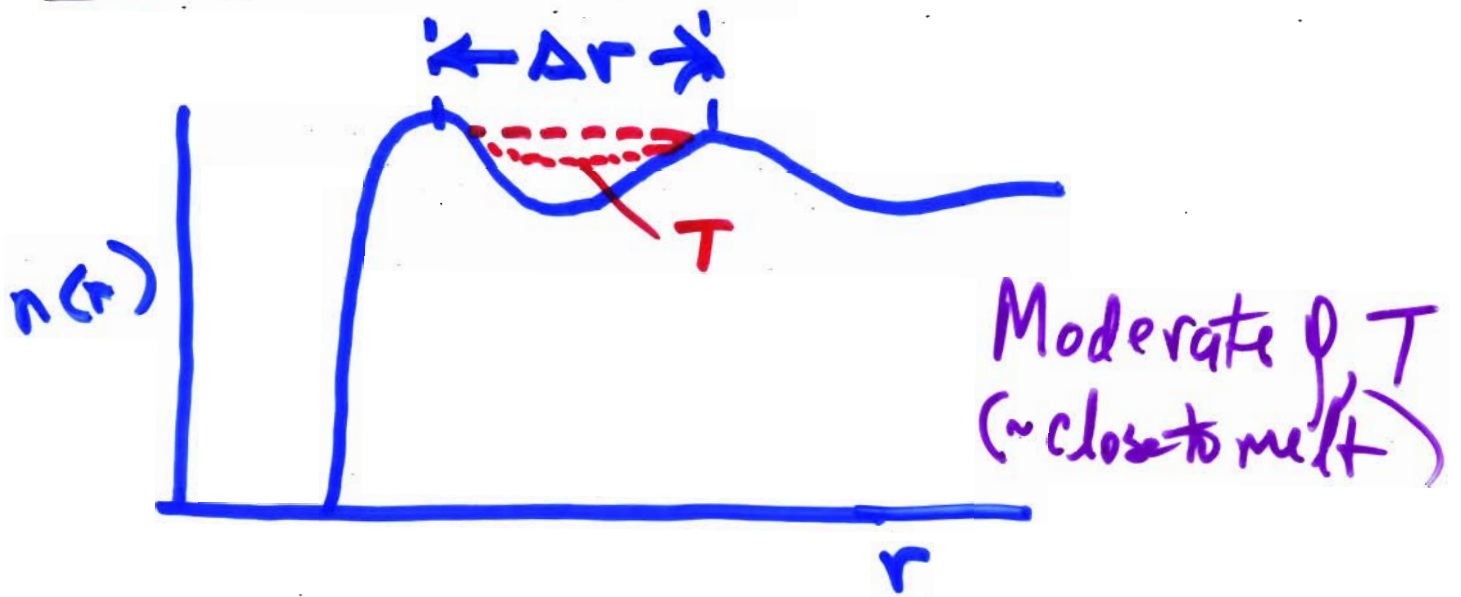
Solid-solid phase transitions, including glass formation, and melting can occur.

Because of the high rate of compression, high densities of lattice defects are generated in ordered solids, which also cause line broadening of xrd.

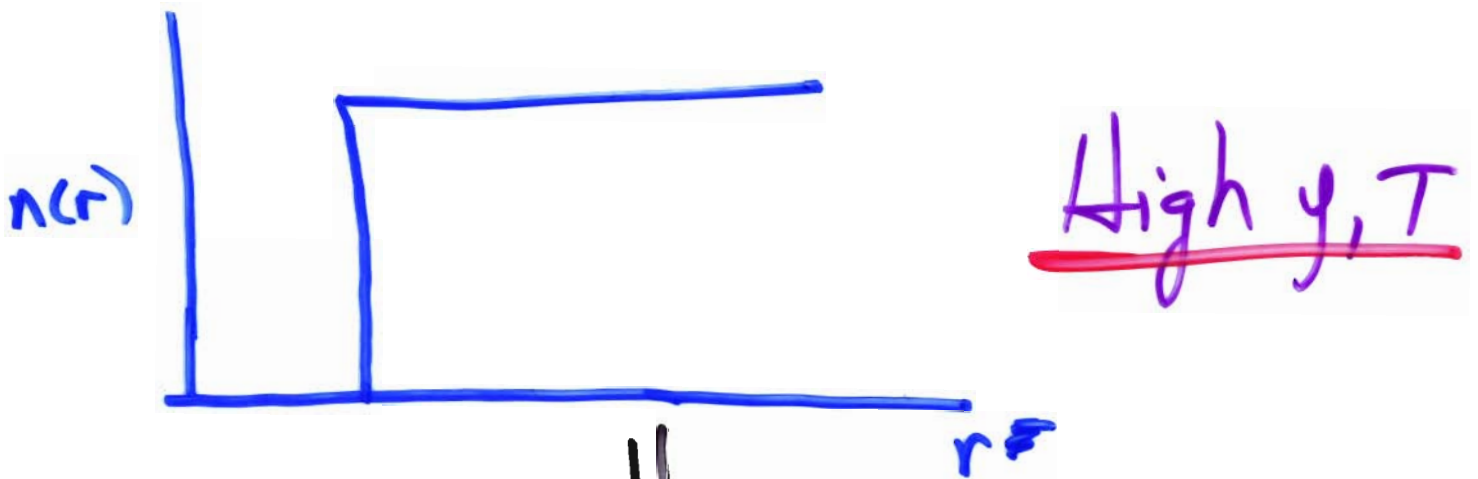




# Pair distributions



$$\Delta r \propto \rho^{1/3} \quad \rho \equiv \text{density}$$



Need theoretical predictions of  $n(r)$  as function of  $\rho, T$  to know where to look

## ERL could be very important to dynamic compression research

Capability to perform X-ray scattering experiments with sufficiently high intensity and short pulses means that structures of disordered materials produced by dynamic compression can be determined *in situ* at extreme conditions.

Only a handful of X-ray diffraction experiments have ever been performed on shock-compressed solids to look at crystal structure.

No X-ray scattering experiment of which I am aware has ever been performed to determine defect structures of shock-compressed ordered solids, nor radial distribution functions of liquids and glasses produced by shock compression.

Thus, *there are great opportunities for ERL coupled with dynamic compression, particularly because dynamic pressure, density and temperature can now be tuned over wide limits.*

## Dense Hydrogen: As important as any material for science and technology

The Holy Grail of **Condensed Matter Physics** - both electrons and protons of  $Z=1$  can be quantum in nature.

Is metallic fluid hydrogen monatomic or diatomic?

How does metallization and dissociation vary with  $T/P$ ?

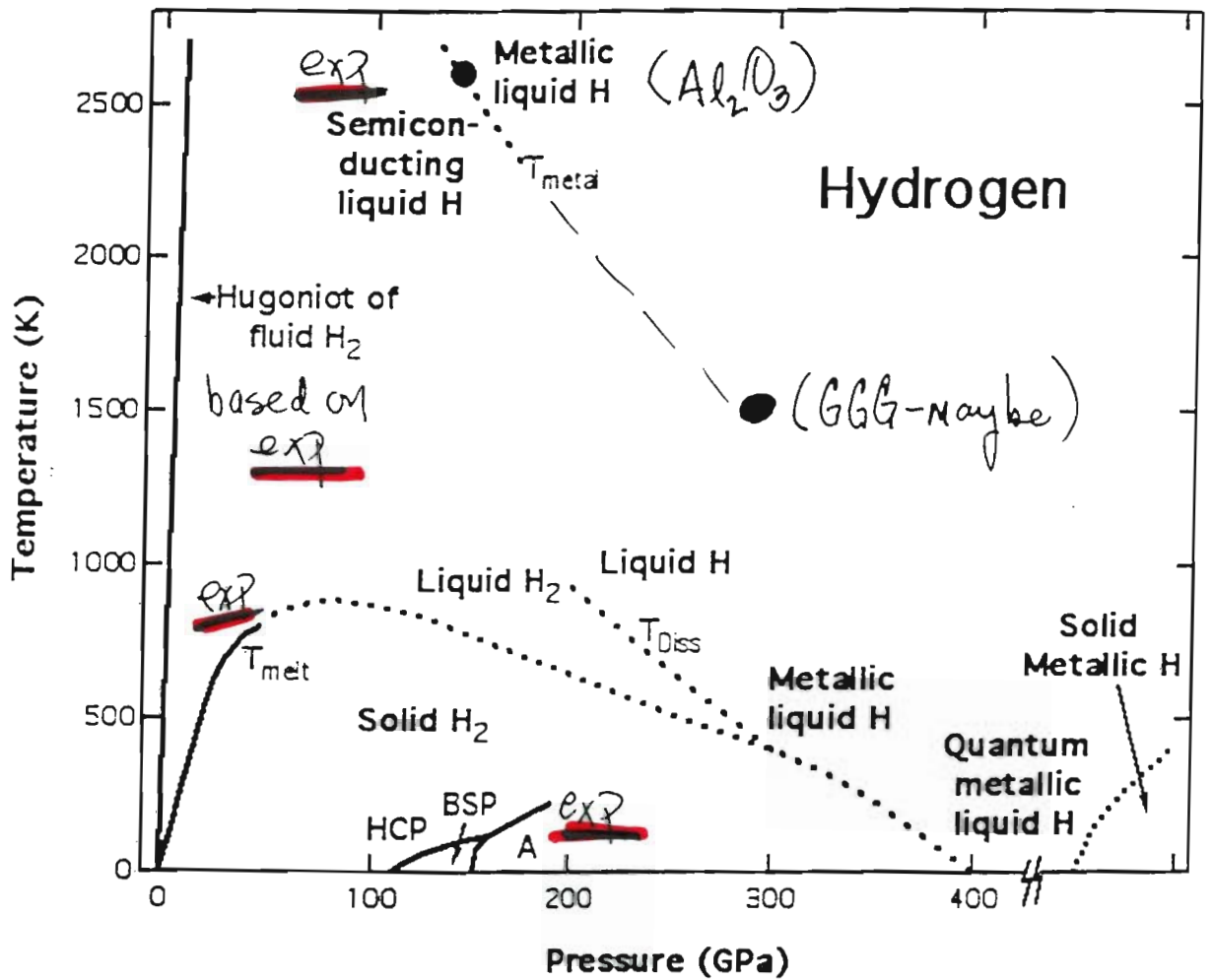
What is  $T_{\text{melt}}(P)$  above 1 Mbar?

Does molecular dissociation play a role in melting?

Physical properties of dense fluid hydrogen must be known to develop pictures of the  $\sim 150$  **giant planets** discovered thus far.

Likewise for **Inertial Confinement Fusion** (40 years of development thus far and 30 more planned-according to NYTimes).

**Metastable solid metallic hydrogen** has innumerable scientific secrets to discover and potential benefits to society. For example, the internal energy in fluid metallic hydrogen at pressure is **120 MJ/kg**, 24 times greater than current hydrogenous materials at ambient (5 MJ/kg).



## Dynamic conditions in hydrogen for ERL

Question: Is fluid metallic hydrogen monatomic or diatomic?

Pressures up to  $\sim 300$  GPa (3 Mbar)

Densities up to  $\sim 12 \rho_{0L}$

Temperatures up to  $\sim 3000$  K

These conditions are achieved by a combination of shock and isentropic compression for  $\sim 100$  ns.

## X-ray scattering and structures

Melting is observed as transition from Xrd to pair distribution function.

Hydrogen structures:

Solid has small Debye-Waller factors and is highly defected.

Pair distribution function of melt must be measured very accurately.

$Z=1$ .

To determine such structures:

ERL gives intense, short ( $\sim$ ps), focused ( $\sim$ 50  $\mu$ m) pulses every  $\sim$ ns for  $\sim$ 100 ns.

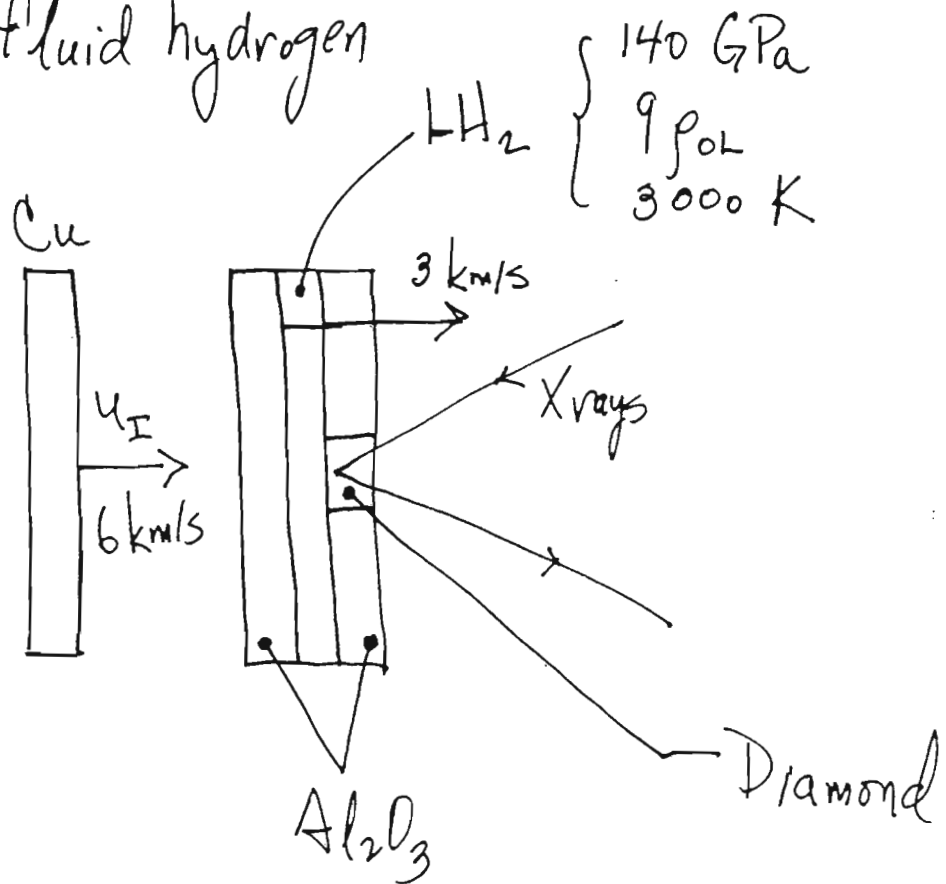
Statistics are improved by multiple irradiations of the same state.

Same steady state is needed for long time ( $\sim$ 100 ns).

Generate dynamic compression with impact of a plate (10 mm in diameter and mm thick) accelerated with two-stage gun ( $<$ 3 m long).

# Measure pair distribution function

Metallic fluid hydrogen





An incompressible material is one for which the slope of shock pressure  $P$  with compression  $\eta$  is very large.

From the Hugoniot equations:

$$(dP/d\eta)_H = \rho_0 u_s^2 [(1+x)/(1-x)]$$

$$x = (u_p/u_s)(du_s/du_p), \text{ where}$$

$\rho_0$  = initial density

$\rho$  = shock-compressed density

$$\eta = \rho/\rho_0$$

$u_p$  = particle velocity

$u_s$  = shock velocity

$(dP/d\eta)_H$  is large for large  $\rho_0$  and  $u_s$   
and for  
 $x \rightarrow 1$  ( $u_s \rightarrow Su_p$  at large  $u_p$ , independent of  $\rho_0$ ).

Phase transitions might cause  $u_s$  to increase faster at high pressures than at low pressures.

Oxides are known to have phase transitions at high shock pressures and TiO<sub>2</sub> and GGG and are more incompressible than diamond at high shock pressures.

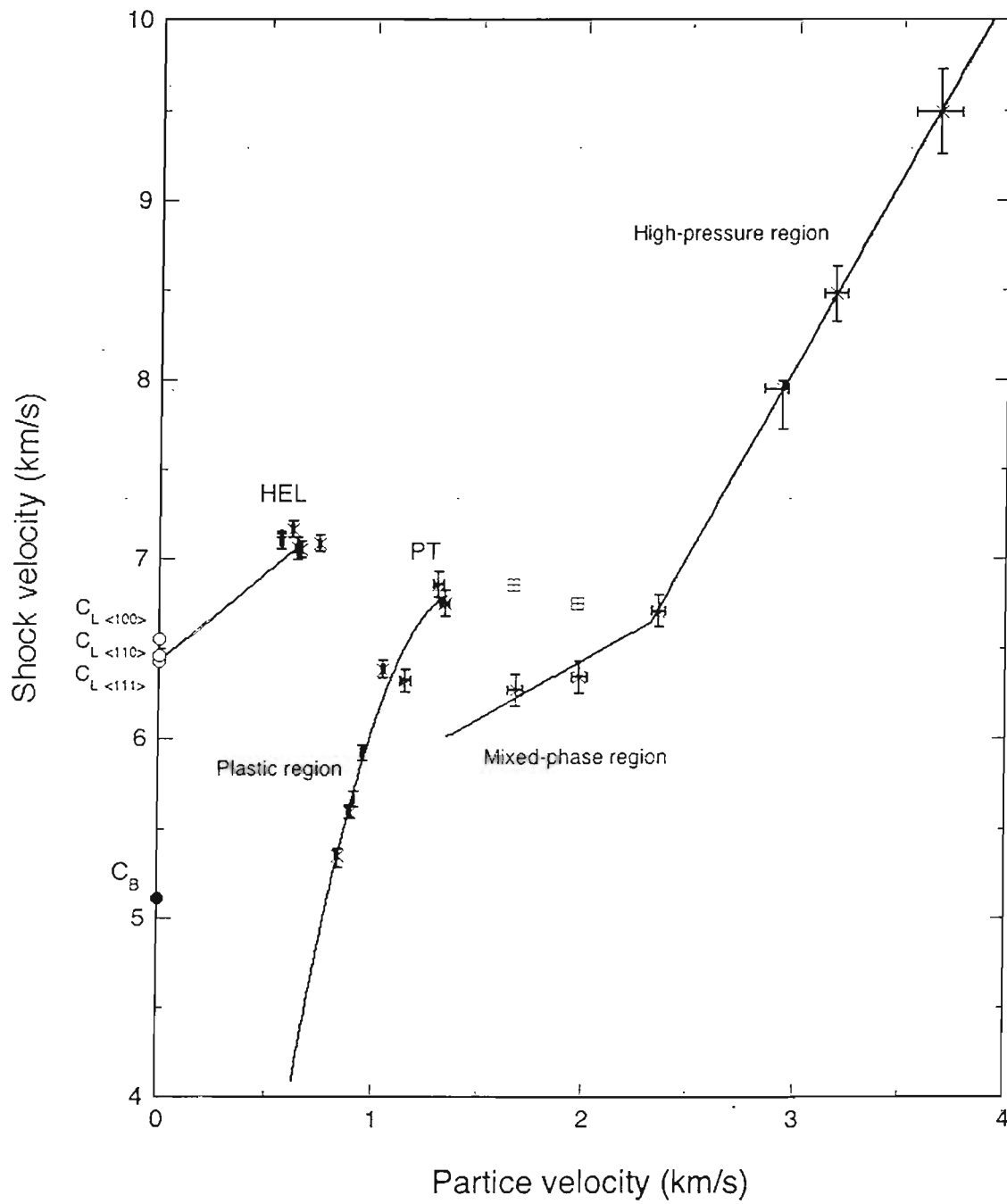


Fig. 1 Mashimo et al.

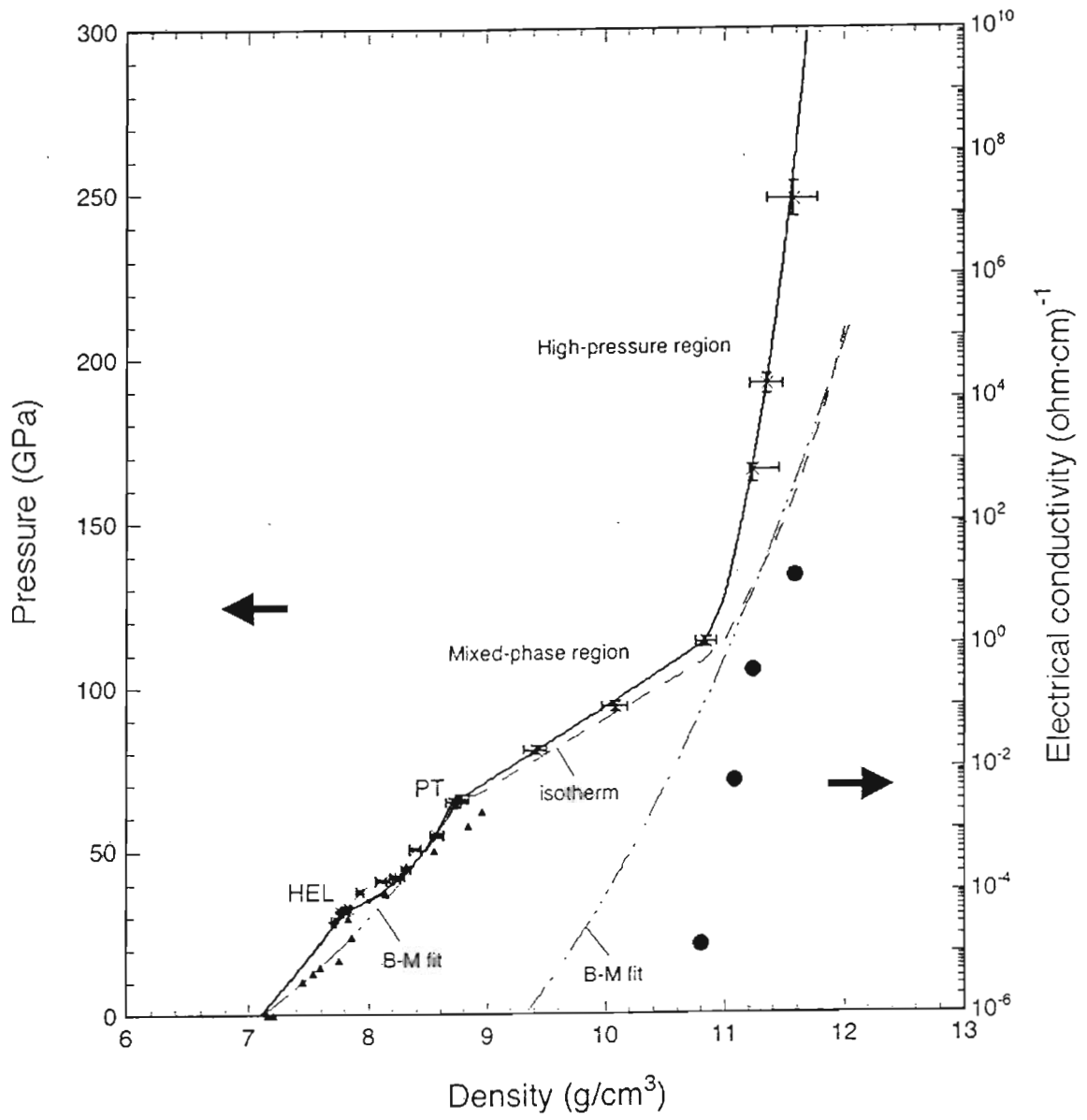


Fig. 2 Mashimo et al.

## GGG Experiment

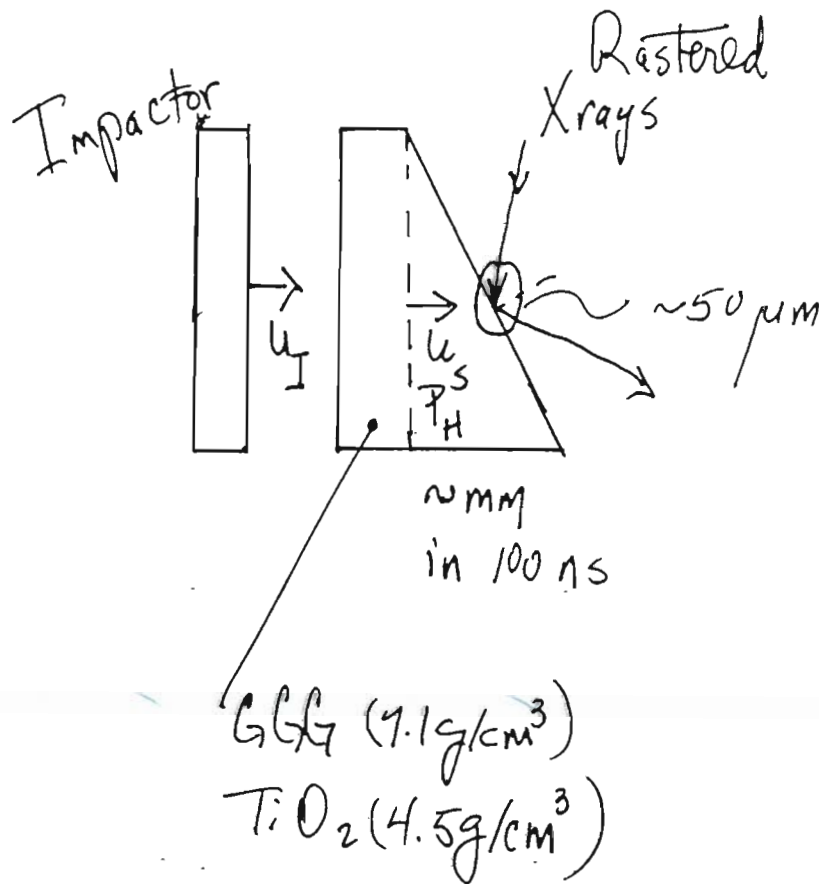
Take advantage of 100 ERL pulses every ns.

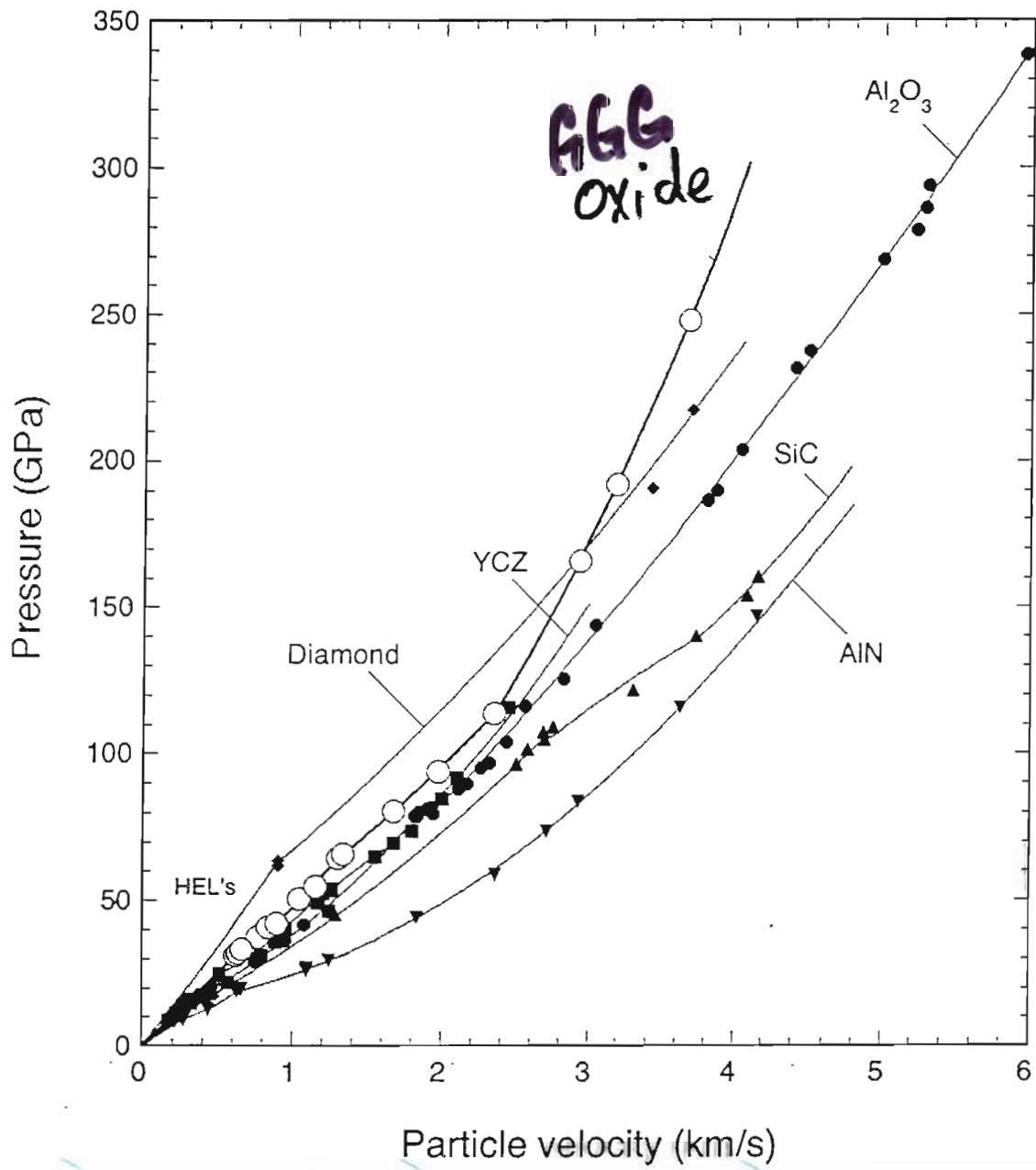
In 100 ns shock front moves  $\sim$ mm.

Optical depth of GGG for X rays is  $\sim$  $\mu$ m.

ERL beam size is  $\sim$ 50  $\mu$ m.

Each pulse must scatter off free surface when shock is within  $\sim$  $\mu$ m of the surface.





GGG is quite complex under shock compression

Elastic-plastic transition at 30 GPa

Phase transition, probably to a glass, at 65 GPa

Transition to an unknown phase less compressible than diamond at 120 GPa

(At ambient GGG has the cubic garnet structure and  $\rho_0=7.1 \text{ g/cm}^3$ .)

## What is the purpose of dynamic compression?

The purpose considered here is to achieve high pressures, densities and modest temperatures in thermally equilibrated condensed matter. That is, for metals  $T/T_F < 1$ .

With quasi-isentropic compression and laser heating of a diamond cell, temperatures achieved by dynamic and static compression approach one another.



P(GPa)

400

300

200

100

1.0

1.1

1.2

1.3

1.4

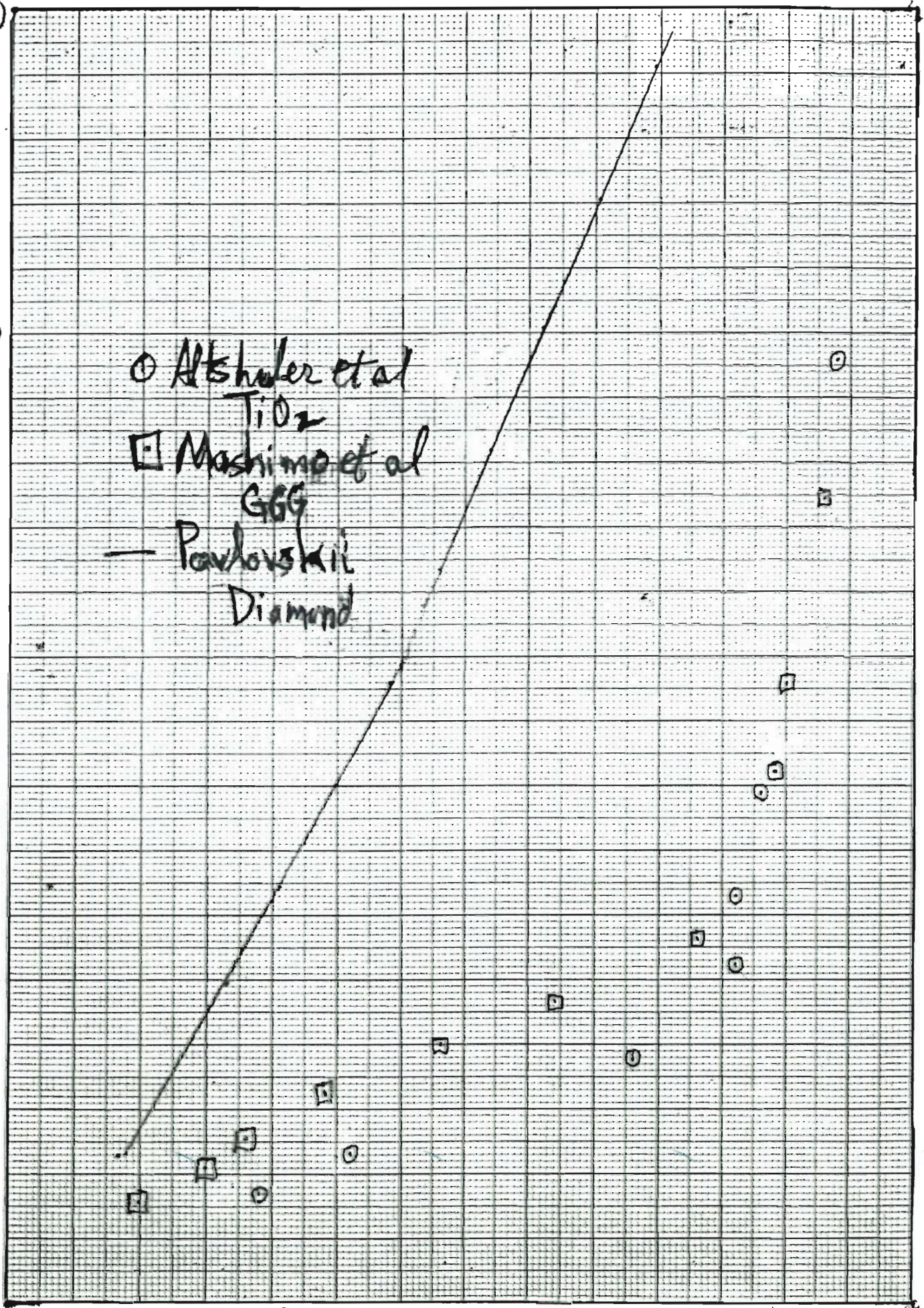
1.5

1.6

1.7

○ Alshuler et al  
TiO2  
 □ Mashimo et al  
GGG  
 — Pavlovskii  
 Diamond

$$\gamma = \frac{P}{V} = 1.2$$





GRAPH PAPER  
Pressure (GPa)

300

200

100

$TiO_2$   
— Debyevoinsky et al (300K)  
--- ○ Atshuler et al (Hydrostat)  
--- △ McQueen et al (Hydrostat)

Diamond Cell

1.0

1.1

1.2

1.3

1.5

1.6

1.7

