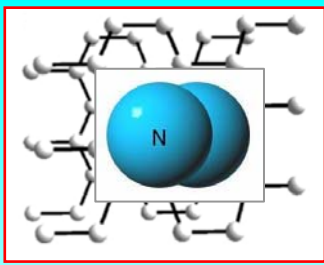


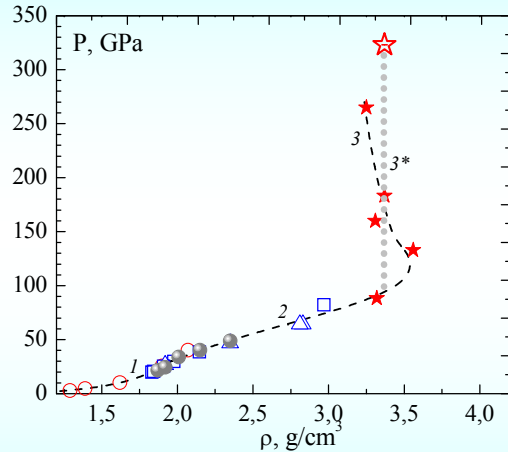


*4th EMMI workshop*  
**Plasma Physics with Intense Heavy Ion and Laser Beams**  
*GSI, Darmstadt, Germany*  
 May 2 - 4, 2011



# Shock compression of liquid nitrogen

Thermodynamic analysis *of new experimental data in megabar range*



**Igor Iosilevskiy**

*Joint Institute for High Temperature (Russian Academy of Science)  
 Moscow Institute of Physics and Technology (State University)*

**Victor Gryaznov, Vladimir Fortov**

*Institute of Problem of Chemical Physics (Russian Academy of Science)*



# Shock compression of liquid nitrogen

*(new experimental data in megabar range)*

1

Mochalov M., Zhernokletov M., Il'kaev R., Mikhailov A., Mezhevov A., Kovalev A., Kirshanov S., Grigorieva Yu., Novikov M., Shuikin A., Fortov V., Gryaznov V., Iosilevskiy I.

*JETP, 137, 77 (2010)*

*Density, temperature and electroconductivity measurements in shock compressed condensed nitrogen at megabar pressure*

2

Trunin R., Boriskov G., Bykov A., Medvedev A., Simakov G., Shuikin A.

*JETP Letters, 88 (3), 189 (2008)*

*Shock compression of condensed nitrogen at megabar pressure*



Collaboration:

*Eugene & Lidia Yakyb*

*(Odessa University, Ukraine)*

# Content

**Experimental data on nitrogen shock compression at  $P \sim 100 - 300$  GPa**

**First comments ( *thermodynamics* )**

**New experimental data as powerful tool to check theoretical models**

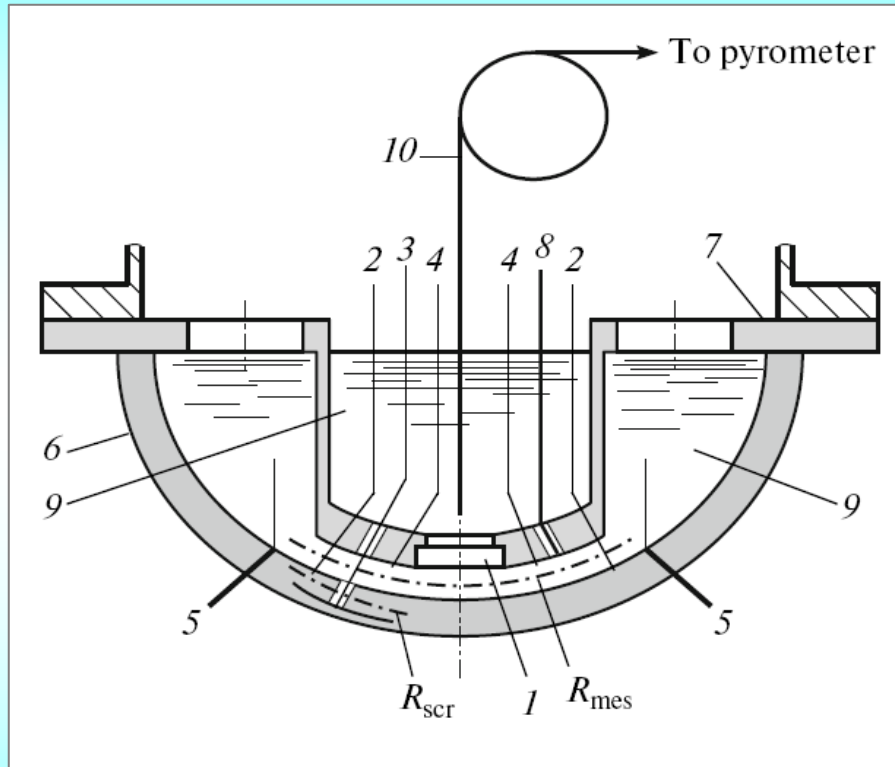
**Plasma model for EOS of nitrogen in megabar range**

**Conclusions *and* perspectives**

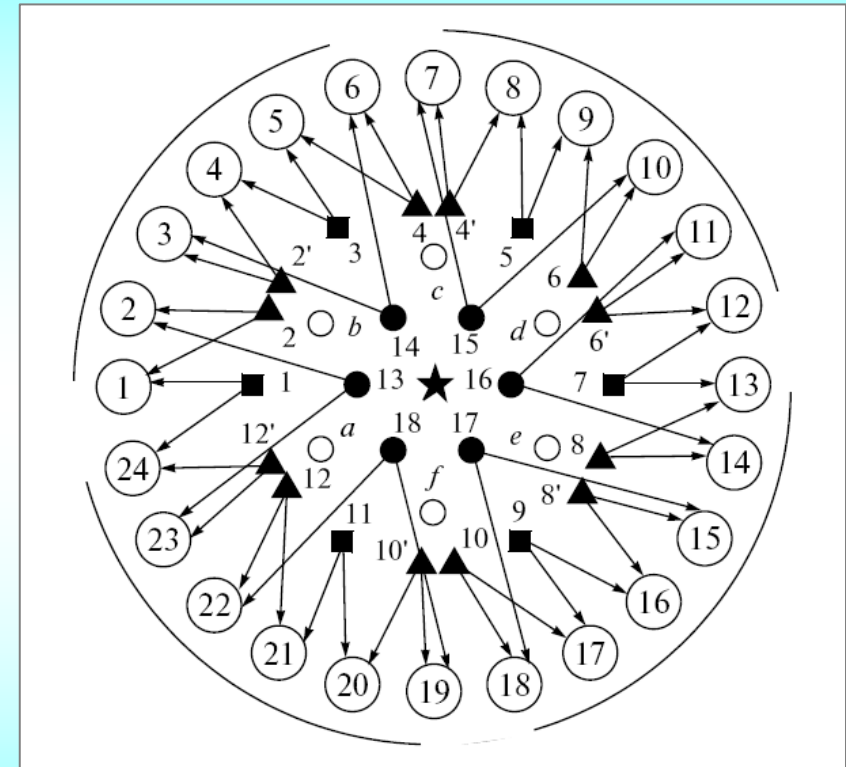
# Experimental setup

## *Semi-spherical explosive shock wave generator*

Mochalov M., Zhernokletov M., et al., *JETP*, **137**, (2010)



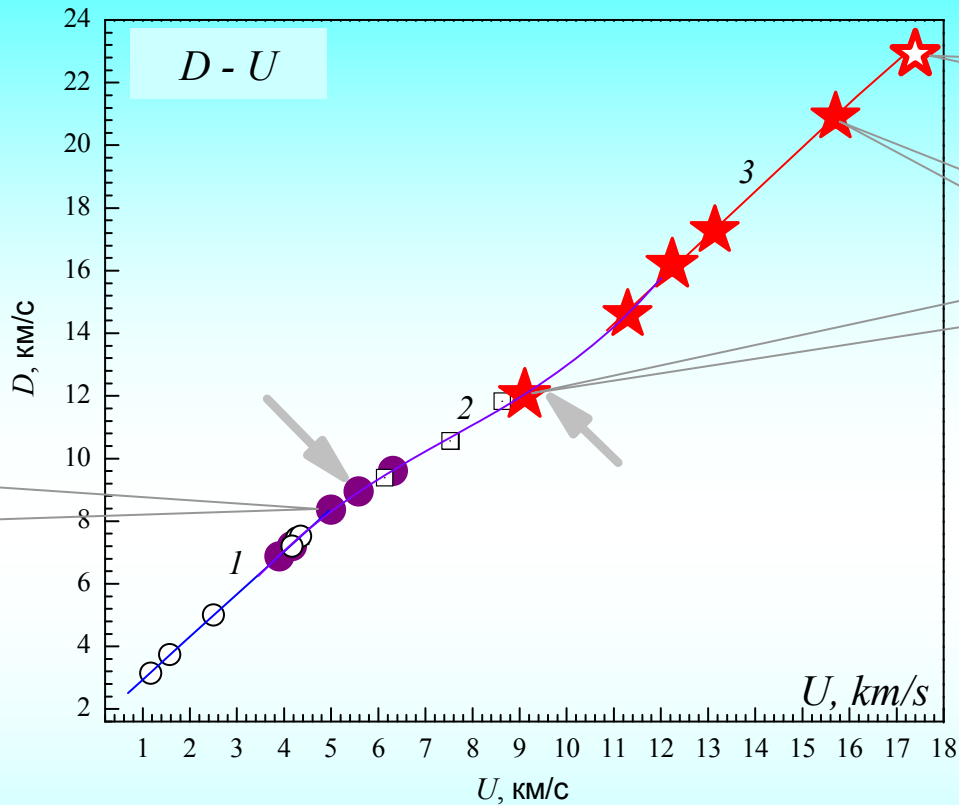
**Fig. 2.** Measuring unit: (1) optical window; (2–5) contacts; (6) screen; (7) holder; (8) optical sensors; (9) liquefied gas; (10) optical fiber.



**Fig. 3.** Schematic of contacts sensors ((■) in the screen, (▲) on the screen surface, and (●) in the nitrogen) and optical ((○) fibers with photodiode, transducers; (★) optical fiber for recording spectral temperatures) sensors in the hemispherical cryogenic unit. Numbers in circles indicate measuring channels.

# Shock Hugoniot of liquid nitrogen

(kinematic variables)



Mochalov et al.  
2010  
(flat geometry)

Trunin et al.  
(2008)

Mochalov et al.  
2010  
(spherical)

$D$	$U$
$12.03 \pm 0.25$	9.11
$14.60 \pm 0.26$	11.29
$16.19 \pm 0.36$	12.24
$17.28 \pm 0.40$	13.14
$20.90 \pm 0.68$	15.71
$22.9 \pm 0.4$	17.4

Initial state  
 $\rho_0 = 0.81$   
( $T_0 = 77$  K)

$D$  and  $U$  – shock and mass velocities  
Arrows – hypothetical transitions between molecular (1),  
polymeric (2) and plasma (3) states

Approximations:  
1:  $D = 1.365 \cdot U + 1.572$   
2:  $D = 3.375 \cdot U - 0.337 \cdot U^2 + 0.015 \cdot U^3 - 2.008$   
3:  $D = 1.407 \cdot U - 1.174$

★ - Mochalov M., Zhernokletov M. et al.,  
*JETF* 137, 77 (2010)

★ - Trunin R., Boriskov G., Bykov A., Medvedev A.  
*JETF Letters*, 88, 220 (2008)

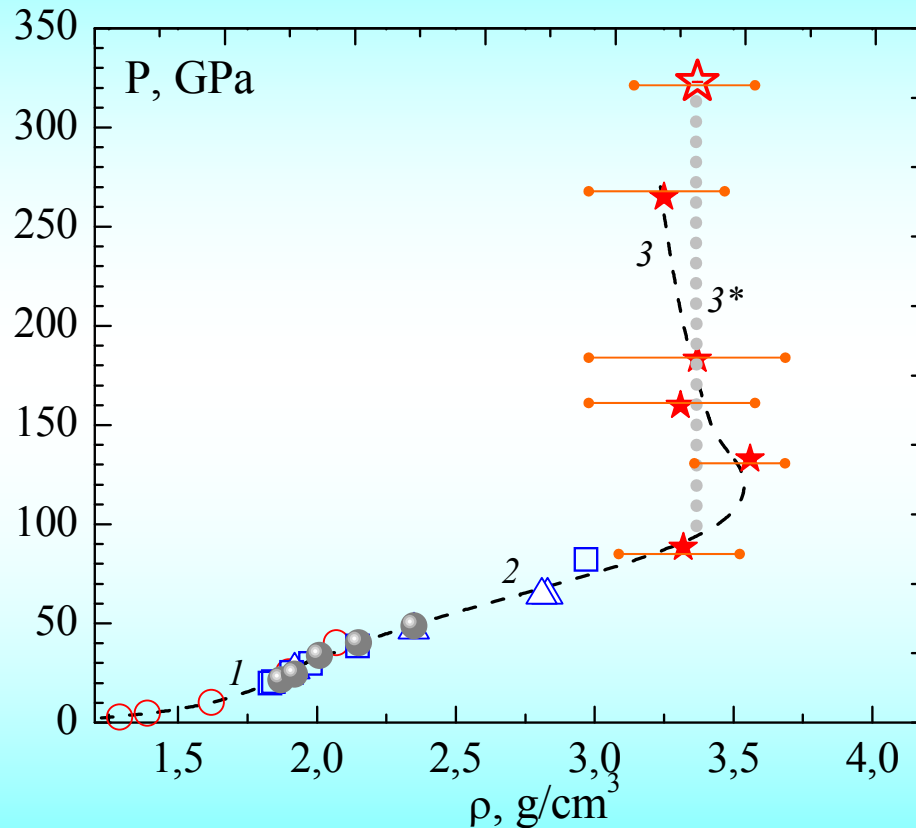
# Shock Hugoniot of liquid nitrogen

(thermodynamic variables)

$$p_1 = p_0 + \rho_0 DU$$

$$h_1 = h_0 + \left( \frac{D^2}{2} - \frac{(D-U)^2}{2} \right)$$

$$\rho_1 = \rho_0 \left\{ \frac{D}{D-U} \right\}$$



$P$ , GPa	$\rho$ , g/cm <sup>3</sup>	$\rho/\rho_0$
$88.4 \pm 2$	$3.325 \pm 0.2$	<b>4.12</b>
$133.3 \pm 3$	$3.56 \pm 0.15$	<b>4.41</b>
$160.0 \pm 3$	$3.31 \pm 0.25$	<b>4.10</b>
$183.0 \pm 3$	$3.37 \pm 0.35$	<b>4.18</b>
$265.0 \pm 5$	$3.25 \pm 0.25$	<b>4.03</b>
323	$3.37 \pm 0.20$	<b>4.16</b>

(\*)  $(\rho/\rho_0)_{\text{ideal gas}} = 4.0$

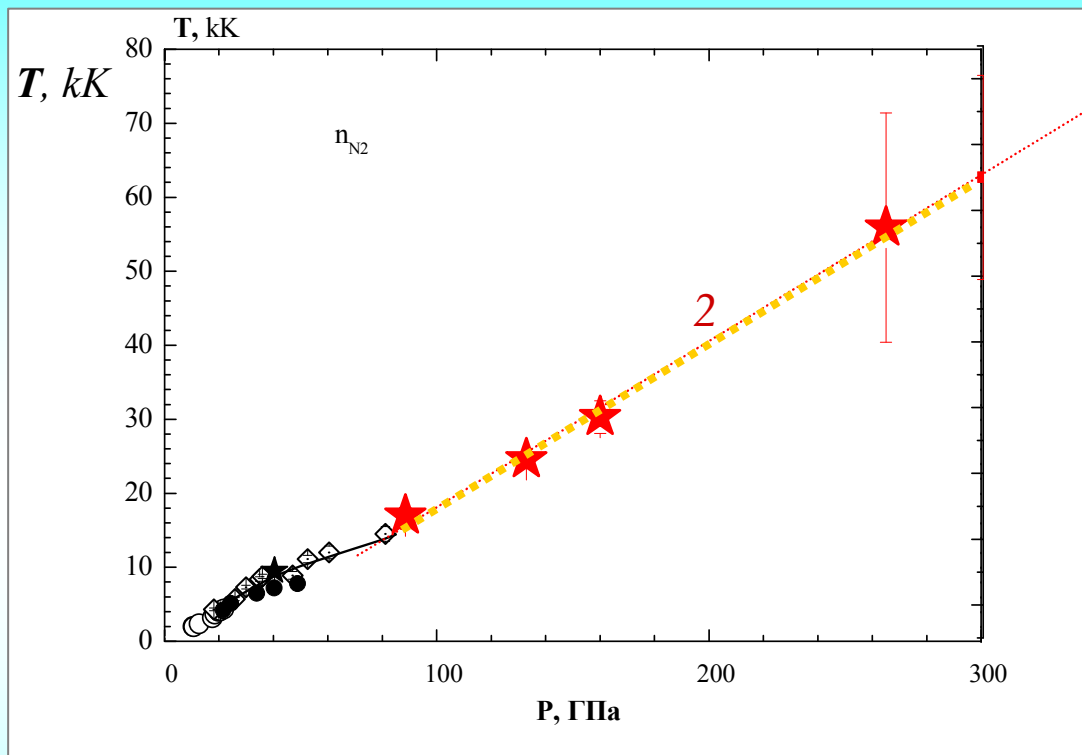
★ - Mochalov M., Zhernokletov M. et al., *JETP* **137**, 77 (2010)

★ - Trunin R., Boriskov G., Bykov A., Medvedev A. *JETP Letters*, **88**, 220 (2008)

# Temperature of shock compressed nitrogen

*measurements of thermal equation of state*

$P$ , GPa	$T$ , kK
$88.4 \pm 2$	$16.2 \pm 0.9$
$133.3 \pm 3$	$24.6 \pm 0.5$
$160.0 \pm 3$	$28.4 \pm 2.2$
$183.0 \pm 3$	-
$265.0 \pm 5$	$56.0 \pm 15.2$
323	-



★ - Experiment (Mochalov M., Zhernokletov M. et al., *JETF* 137, 77 (2010))

2 - linear approximation of experimental data ( $P \approx 90 - 300$  ГПа)

# **Comments**

*phenomenology*

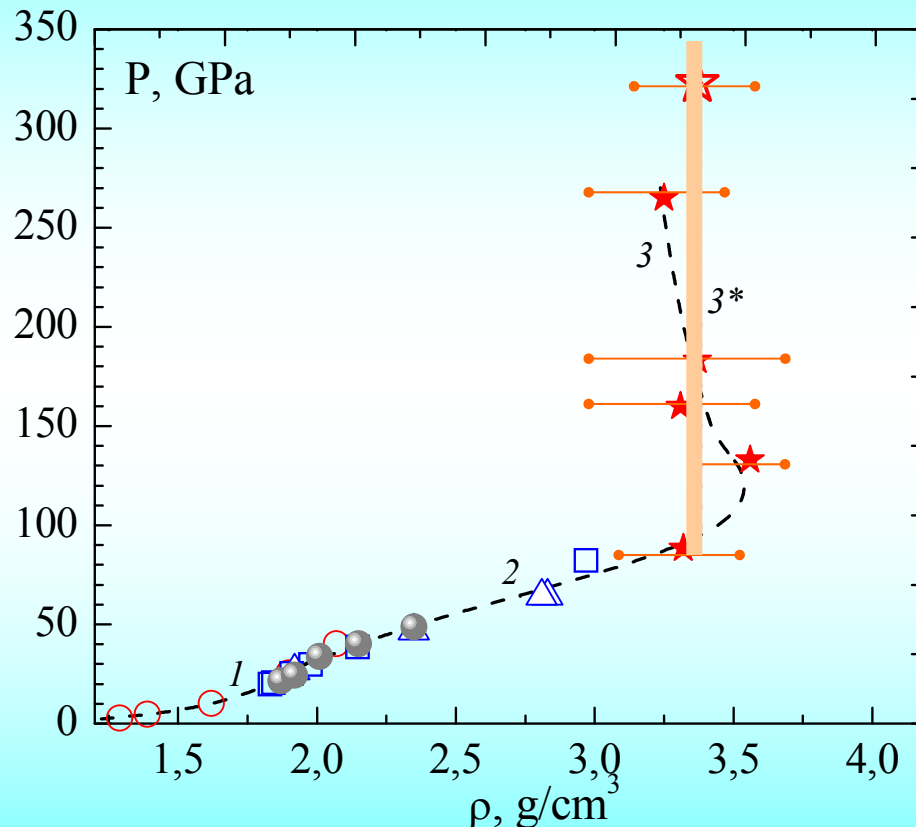


# Nitrogen Hugoniot is close to isochore

$$p_{\text{Hug}} \approx 90 \div 350 \dots \text{GPa}$$



$$\rho_{\text{Hug}} \approx 3.3 \dots \text{g/cm}^3 \approx \text{const}$$



$$\rho_1 = \rho_0 \left\{ \frac{D}{D-U} \right\}$$

$$p_1 = p_0 + \rho_0 D U$$

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★ - Mochalov M., Zhernokletov M. et al., *JETP* **137**, 77 (2010)

★ - Trunin R., Boriskov G., Bykov A., Medvedev A. *JETP Letters*, **88**, 220 (2008)

# Nitrogen Hugoniot

M. Ross & F. Rogers

PHYSICAL REVIEW B 74, 024103 (2006)  
MARVIN ROSS AND FORREST ROGERS

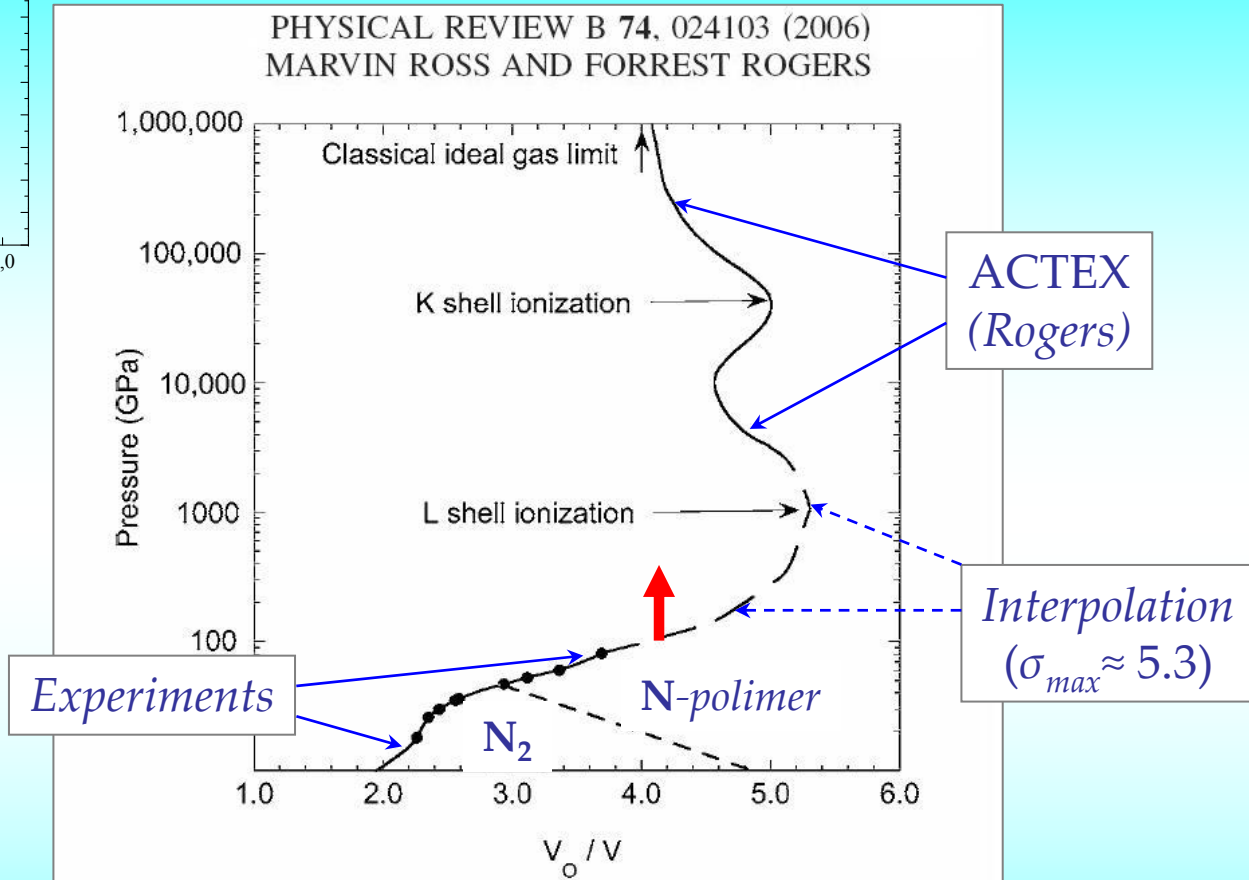
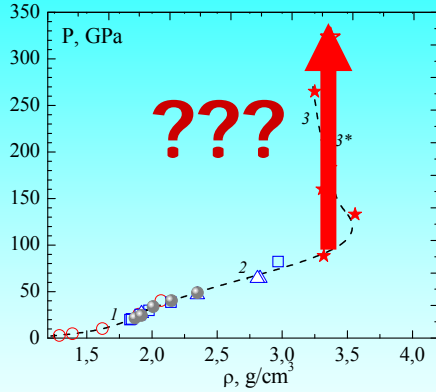
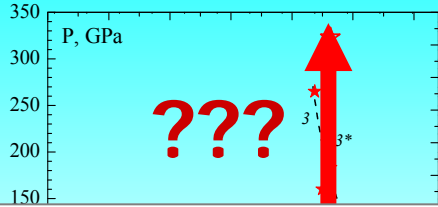


FIG. 6. Nitrogen Hugoniot calculated to extreme conditions, plotted as pressure versus compression ( $V_0/V$ ).  $V_0$  is the initial liquid volume. Experimental data (filled circles) (Ref. 11), connected to ACTEX calculations (solid curve) by a smoothed interpolation (long-dashed curve). The small dashed line locates approximately the liquid molecular-polymer transition.

# Nitrogen Hugoniot

M. Ross & F. Rogers

PHYSICAL REVIEW B 74, 024103 (2006)  
MARVIN ROSS AND FORREST ROGERS



## New experiments ?

- Shock waves
- Heavy Ion Beams
- Laser Heating
- ..... etc. etc.

## THEORY ?

Ab initio

RPIMC, DPIMC

DFT/MD

Chem. models

SAHA-S

SAHA-N

.....

WZ-cell models

TFC, MHFS, ...

.....

Wide-range EOS

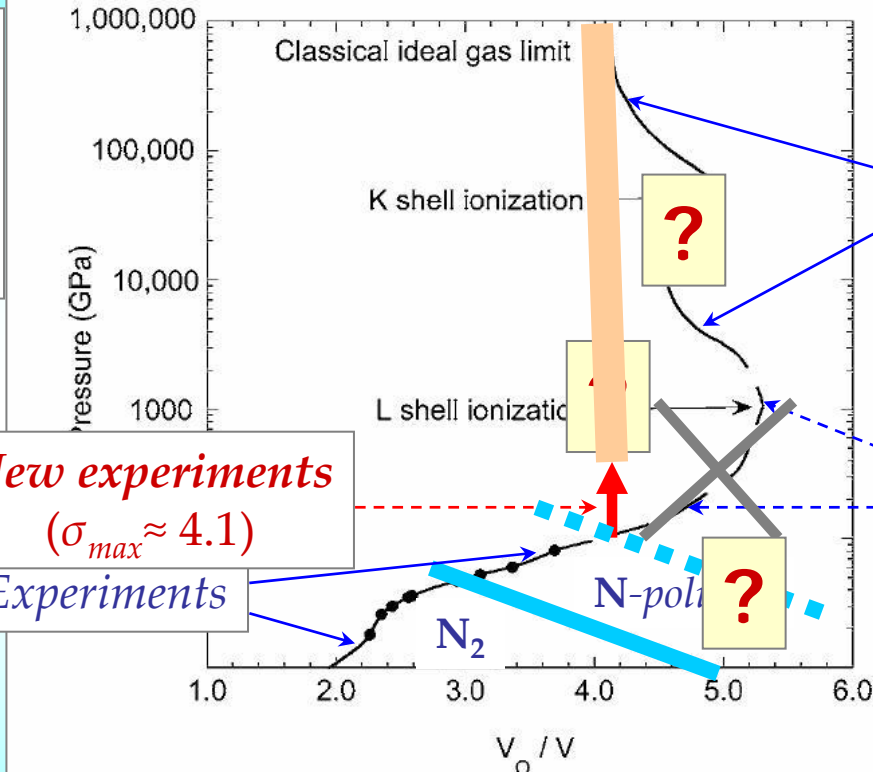
CCM (Sarov)

.....

New experiments

( $\sigma_{max} \approx 4.1$ )

Experiments



ACTEX  
(Rogers)

Interpolation  
( $\sigma_{max} \approx 5.3$ )

**NB !**

FIG. 6. Nitrogen Hugoniot calculated to extreme conditions plotted as pressure versus compression ( $V_0/V$ ).  $V_0$  is the initial liquid volume. Experimental data (filled circles) (Ref. 11), connected to ACTEX calculations (solid curve) by a smoothed interpolation (long-dashed curve). The small dashed line locates approximately the liquid molecular-polymer transition.

In last experiments on deuterium shock compression:

$P_{max} \approx 18$  Mbar

(Mochalov et al. JETP Lett. 2010)

# Comments

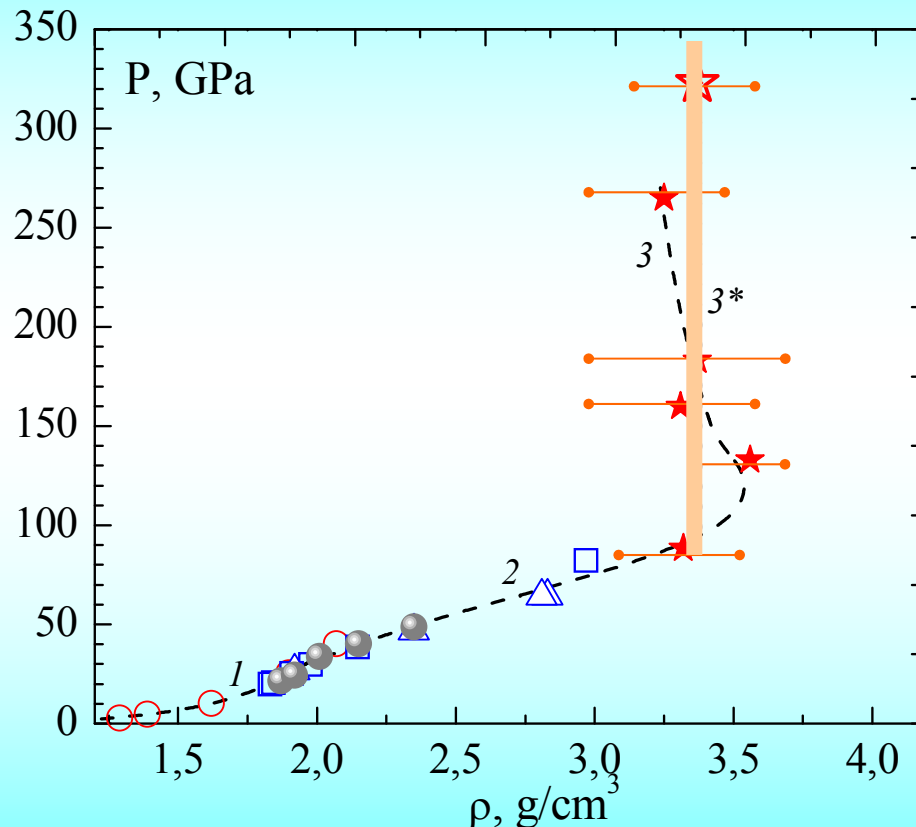
*thermodynamics*

# Nitrogen Hugoniot is close to isochore

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★ - Mochalov M., Zhernokletov M. et al., *JETP* **137**, 77 (2010)

★ - Trunin R., Boriskov G., Bykov A., Medvedev A. *JETP Letters*, **88**, 220 (2008)

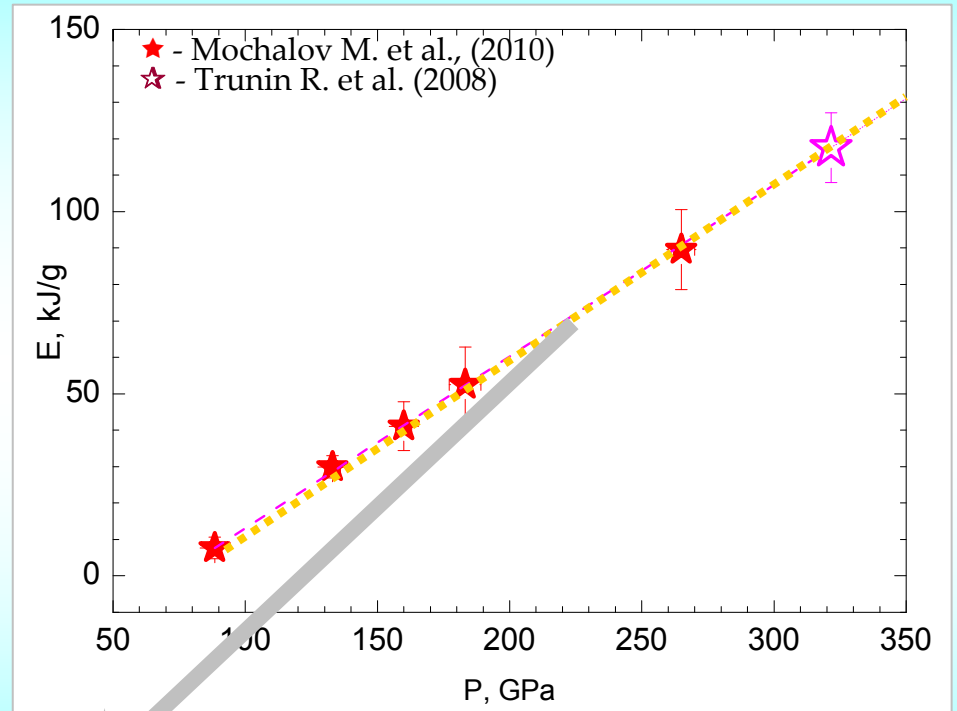
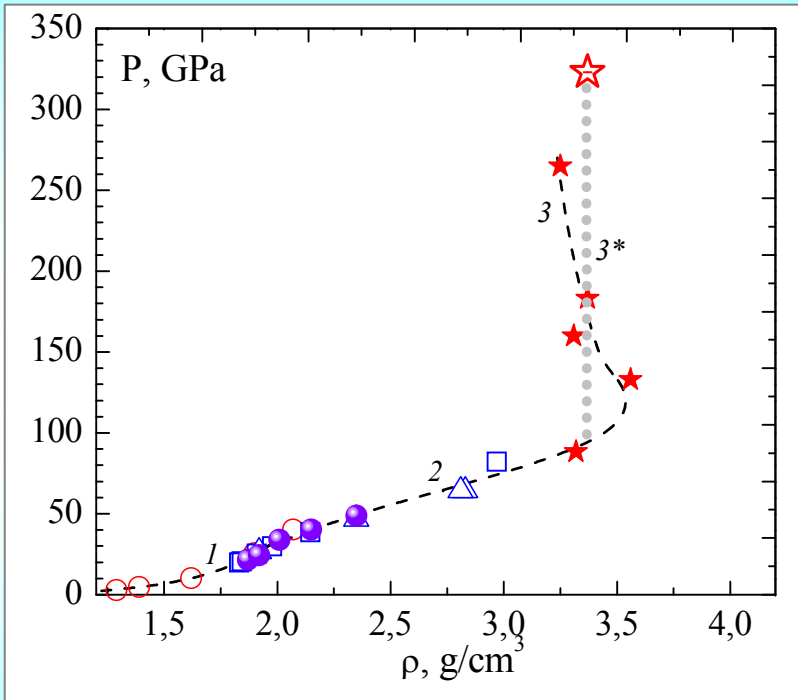
# Internal energy is close to be linear function of pressure

$$E_1 = E_0 + \frac{1}{2} \left( \frac{1}{\rho_0} - \frac{1}{\rho_1} \right) (p_1 + p_0)$$

Approximately linear function:  $E \sim E_0 + \text{const} \cdot P$

Hugoniot:  $\sim \rho \approx \text{const}$  ( $3.3 \pm 0.1$  g/cc)

Internal Energy  $\Leftrightarrow$  Pressure of sock compressed nitrogen



**NB !**

$$\text{Gr} = V(\partial P / \partial E)_V \approx \text{const} \approx 0.62$$

(\*)  $E(P, T)$  reference point – energy of ideal atomic gas N at  $T = 0$  K

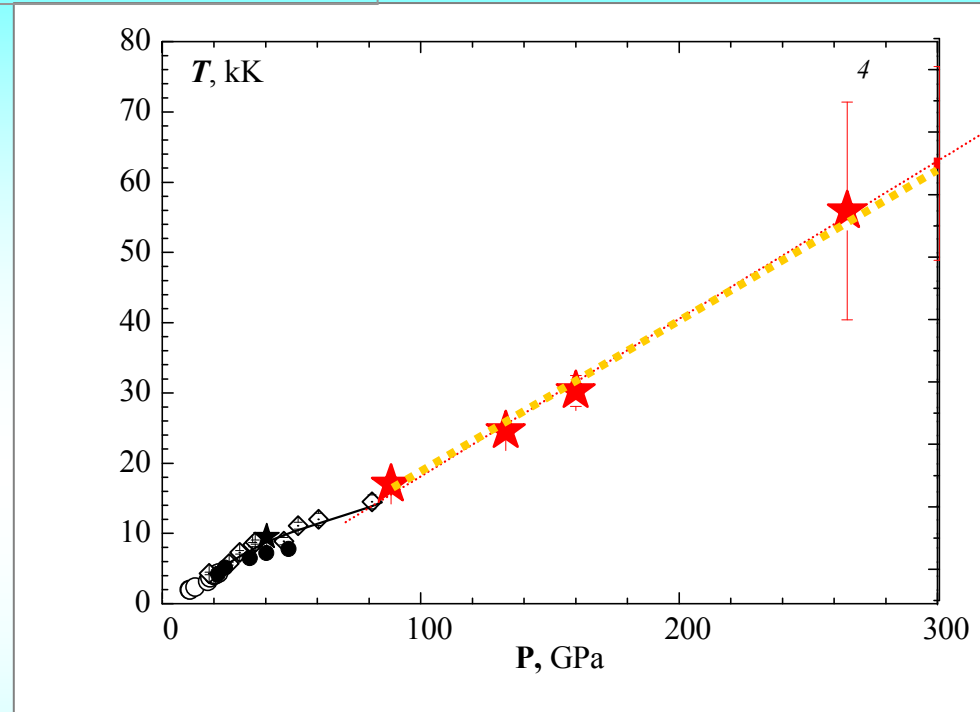
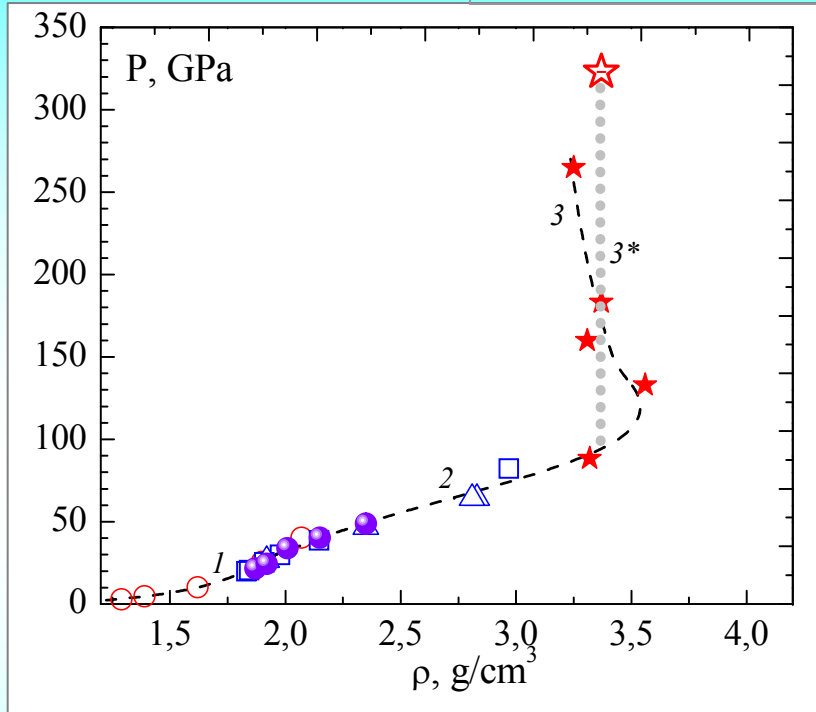
$$(*) \text{Gr}_{\text{id.gas}} = 2/3 \approx 0.67$$

**What does it mean ?**

The region of approximate constancy for Gruneisen parameter  $\Leftrightarrow \rho \approx 3.3 \pm 0.1$  g/cc  $90 < P < 330$  GPa

# Temperature is close to be linear function of pressure + isochoric behavior of nitrogen Hugoniot

$\rho \approx 3.3 \pm 0.1 \text{ g/cc}$  (90 < P < 330 GPa)



★ - Mochalov et al., *JETP* (2010)

**Compressibility factor ( $PV/RT$ ) is almost constant on nitrogen isochore**

**NB !**

$$Z \equiv PV/RT \equiv P/n_N kT \approx \text{const} \approx 2.66 \pm 0.20$$

**What does it mean ?**

$PV/RT$

Ideal gas N<sub>2</sub>: Z= 0.5

Ideal gas N: Z= 1.0

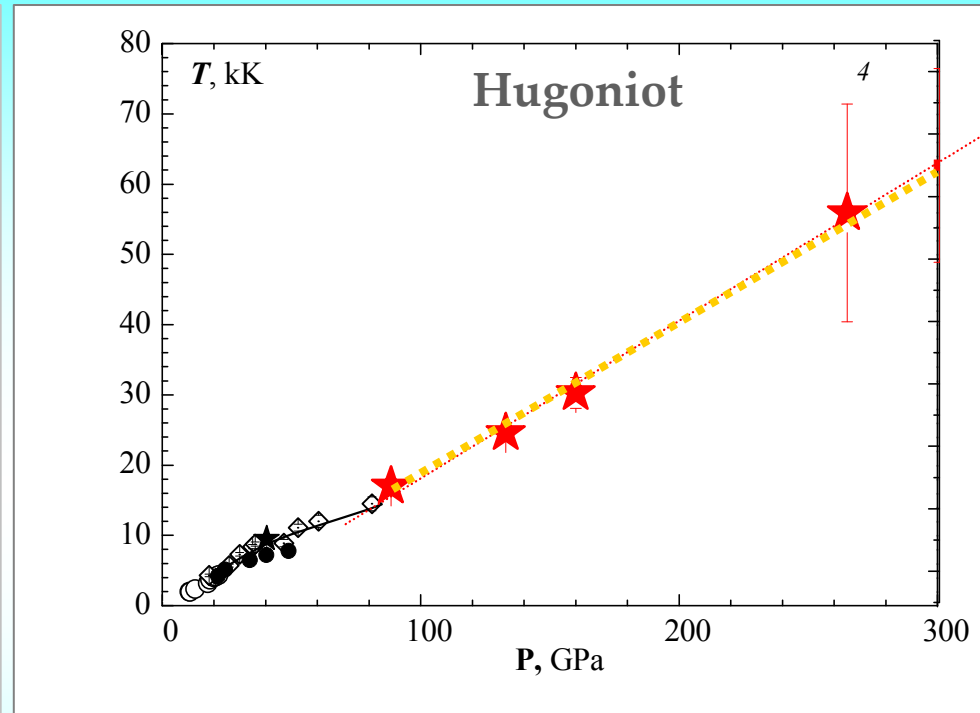
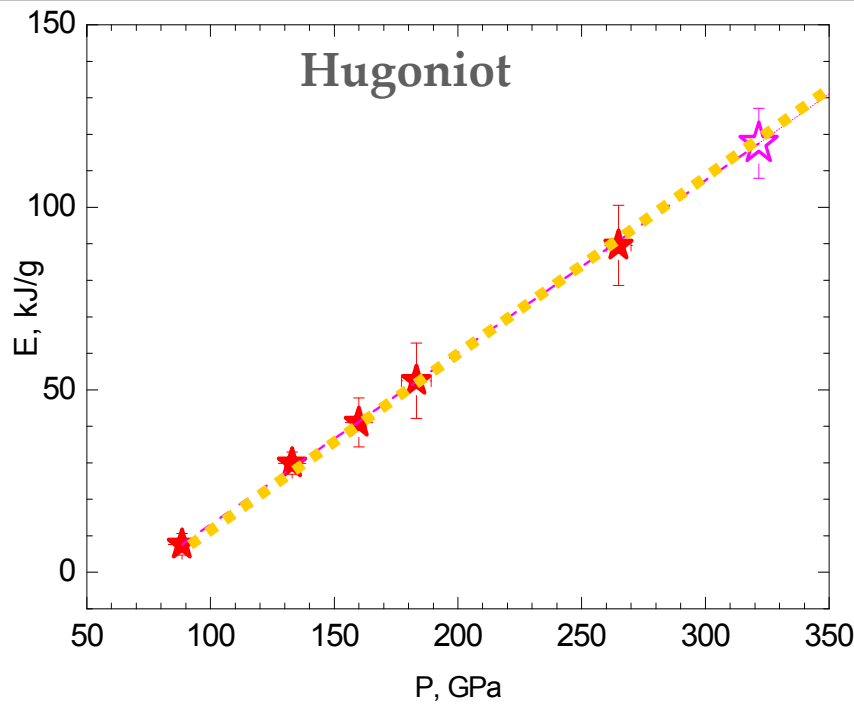
Id. gas N<sup>+</sup> + e: Z= 2.0

.....

## High-temperature part of nitrogen Hugoniot

# Internal energy ~ linear function on temperature at isochore

$$\rho \approx 3.3 \pm 0.1 \text{ g/cc} \quad (90 < P < 330 \text{ GPa})$$



Isochoric heat capacity ( $C_V$ ) is almost constant on nitrogen isochore

**NB !**

$$C_v \equiv (\partial E / \partial T)_v \approx \text{const} \approx 2.0 \text{ (J/gK)}$$

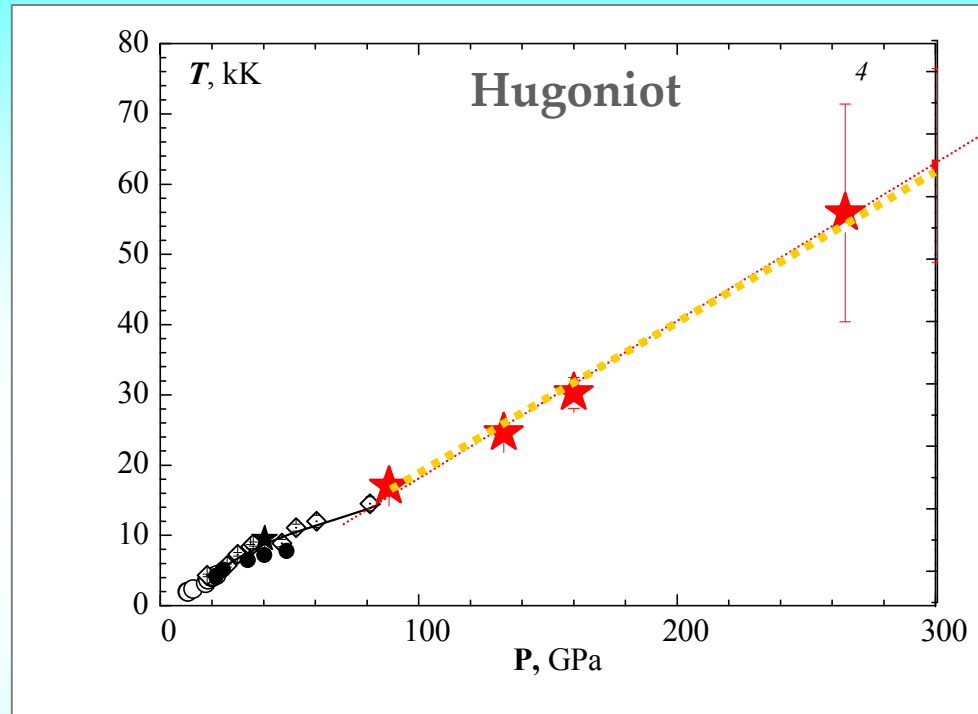
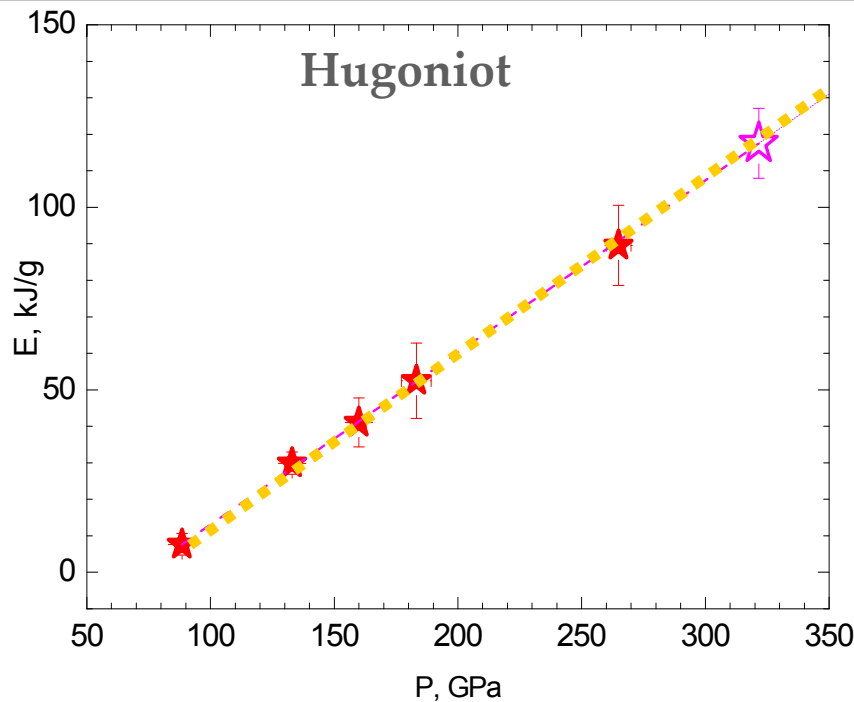
$$C_V / R_N \approx 3.5 !$$

What does it mean ?



# Constancy of Grüneisen parameter *and* Heat capacity at isochore

$$\rho \approx 3.3 \pm 0.1 \text{ g/cc} \quad (90 < P < 330 \text{ GPa})$$



$$Gr \approx const + C_V \approx const \Leftrightarrow \text{thermal pressure coefficient } \gamma_v^* \approx const$$

**NB !**

$$(\partial p / \partial T)_v \approx 4.54 \text{ GPa/K} !$$

$$\gamma_v^* \equiv (v/k_B) (\partial p / \partial T)_v \approx const \approx$$

## Summary

# Thermodynamics of shock compressed nitrogen

*(primary thermodynamic results of experiment)*

High-temperature part nitrogen Hugoniot is close to be isochoric

$$\rho \approx 3.3 \pm 0.1 \text{ g/cc} \quad (90 < P < 330 \text{ GPa})$$

Internal energy is almost linear on pressure at isochores

$$\text{Gr} = V(\partial P/\partial E)_V \approx \text{const} \approx 0.62$$

Temperature is almost linear on pressure at isochores

$$(\partial p/\partial T)_V \approx \text{const} \approx 4.54 \text{ (GPa/K)}$$

$$Z \equiv PV/RT \equiv P/n_N kT \approx \text{const} \approx 2.66 \pm 0.20$$

Internal energy is almost linear on temperature at isochores

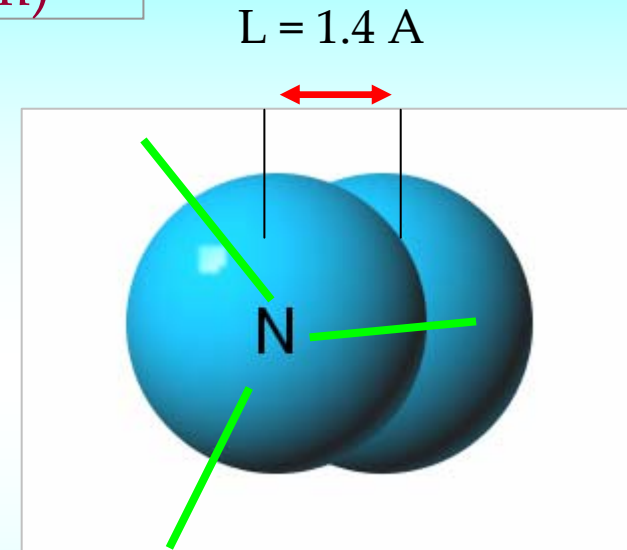
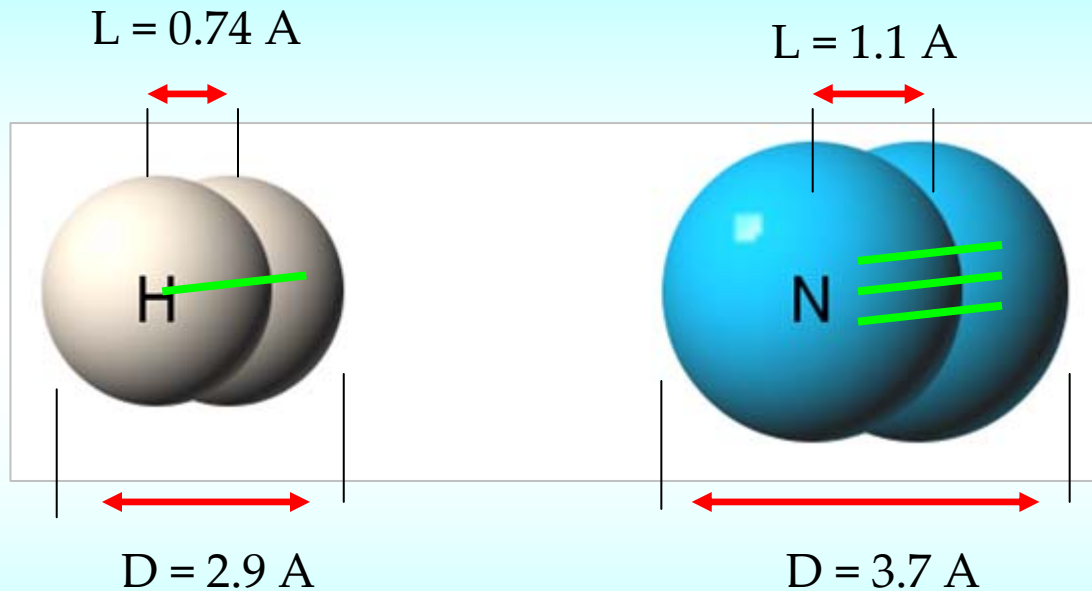
$$C_V \equiv (\partial E/\partial T)_V \approx \text{const} \approx 2.06 \text{ (J/g}\cdot\text{K)}$$

**Comments**

*microphysics*

# Simple molecules: $\text{H}_2 \rightleftharpoons \text{N}_2$

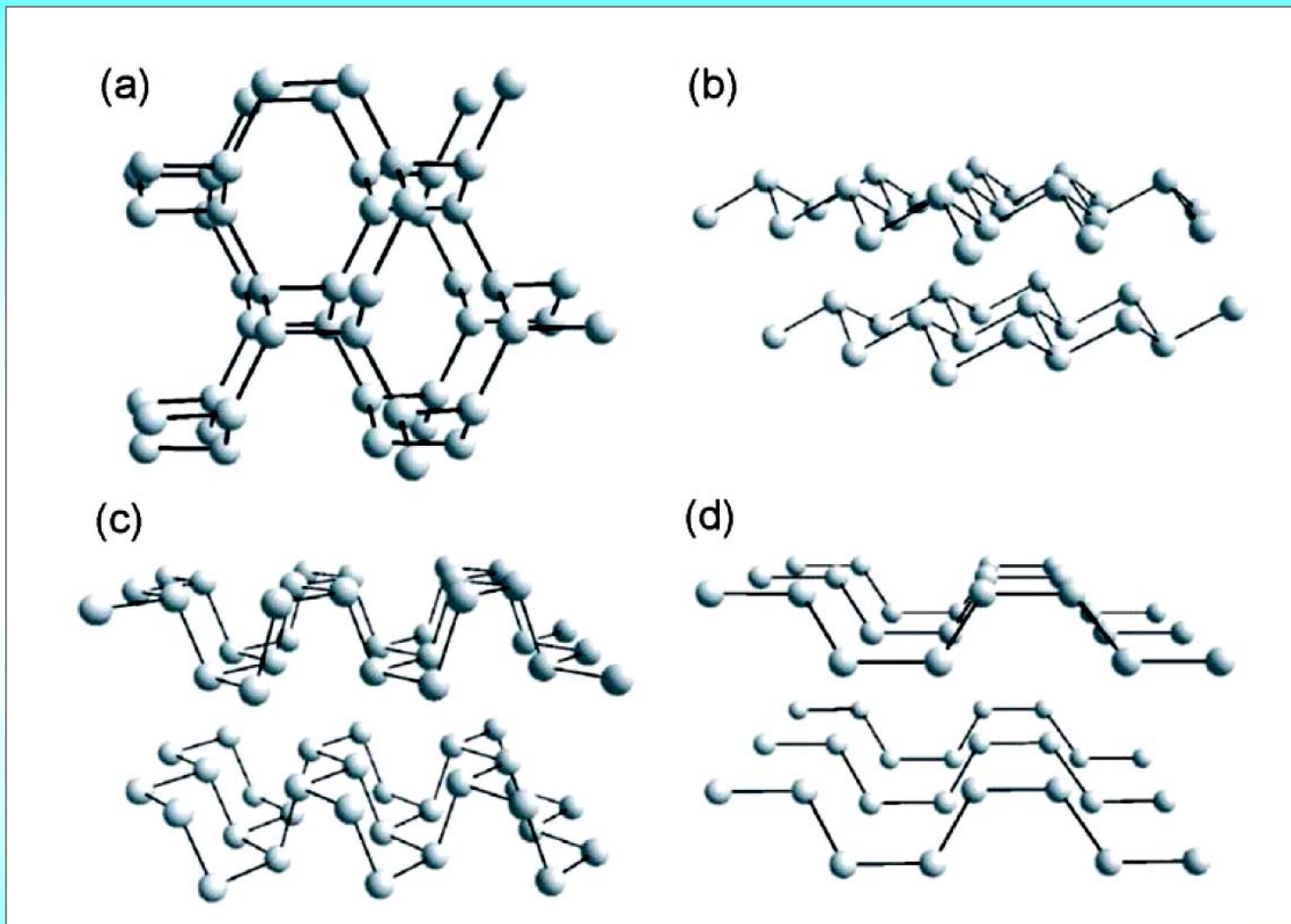
Triple covalent bond  
 $D_e = 9.8 \text{ eV}$  (4.9 eV/atom)



Single covalent bond  
 $D_e = 3.0 \text{ eV}$  (4.5 eV/atom)

Figures after Eugene Yakub: "Non-simple problems for simple molecules"  
FAIR-Russia School «*Physics of high energy density in matter*» December 2009, Moscow

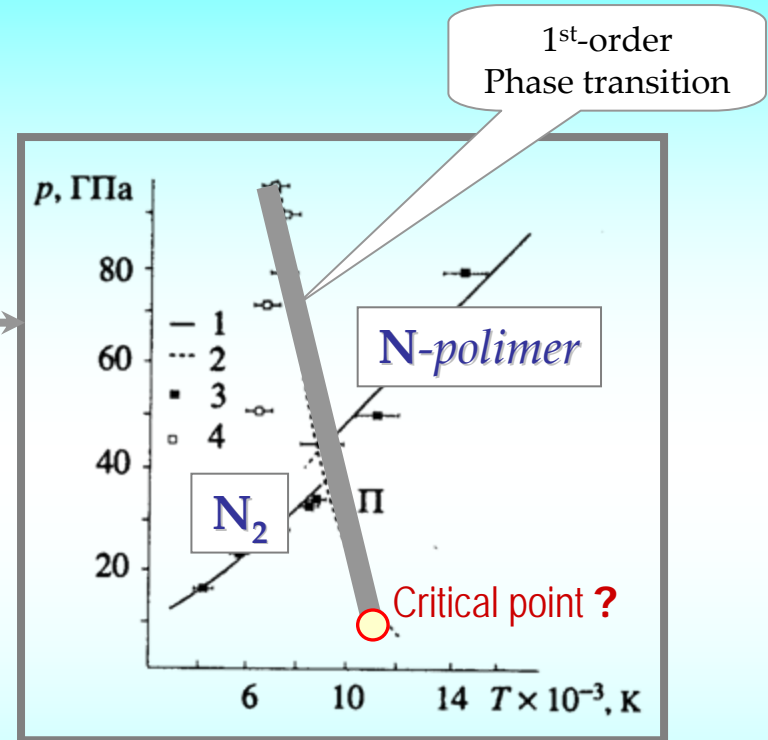
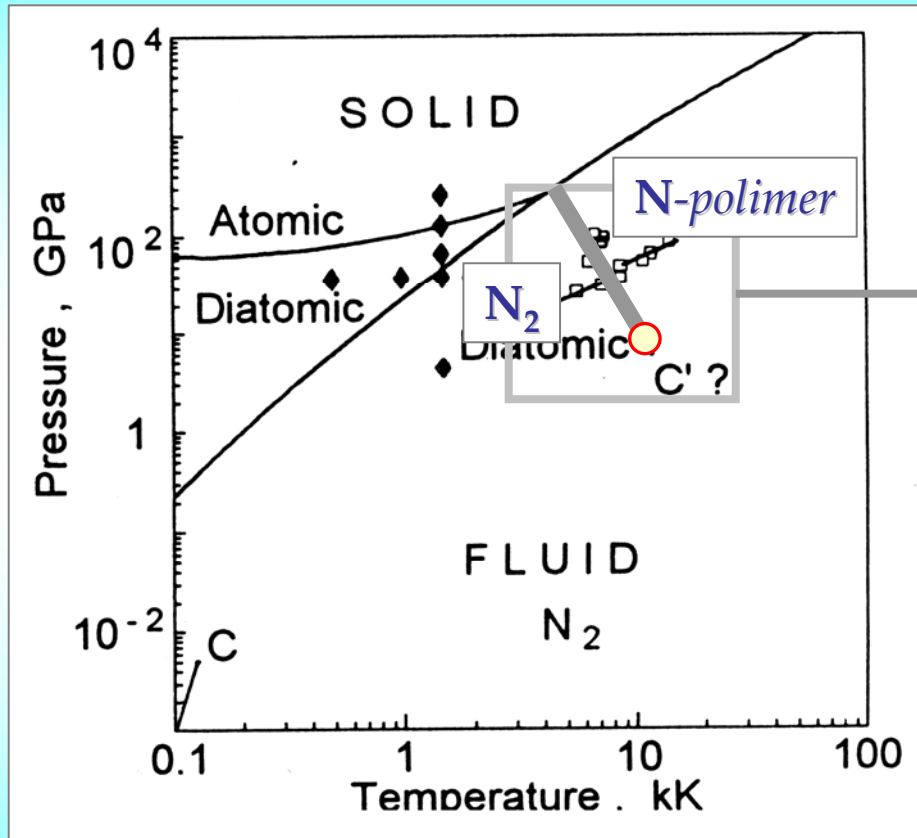
# *Polymeric nitrogen structure*



F.Zahariev,A.Hu,J.Hooper,F.Zhang,&T.Woo. Phys.Rev. B 72,214108 (2005 )

# Simple molecular models

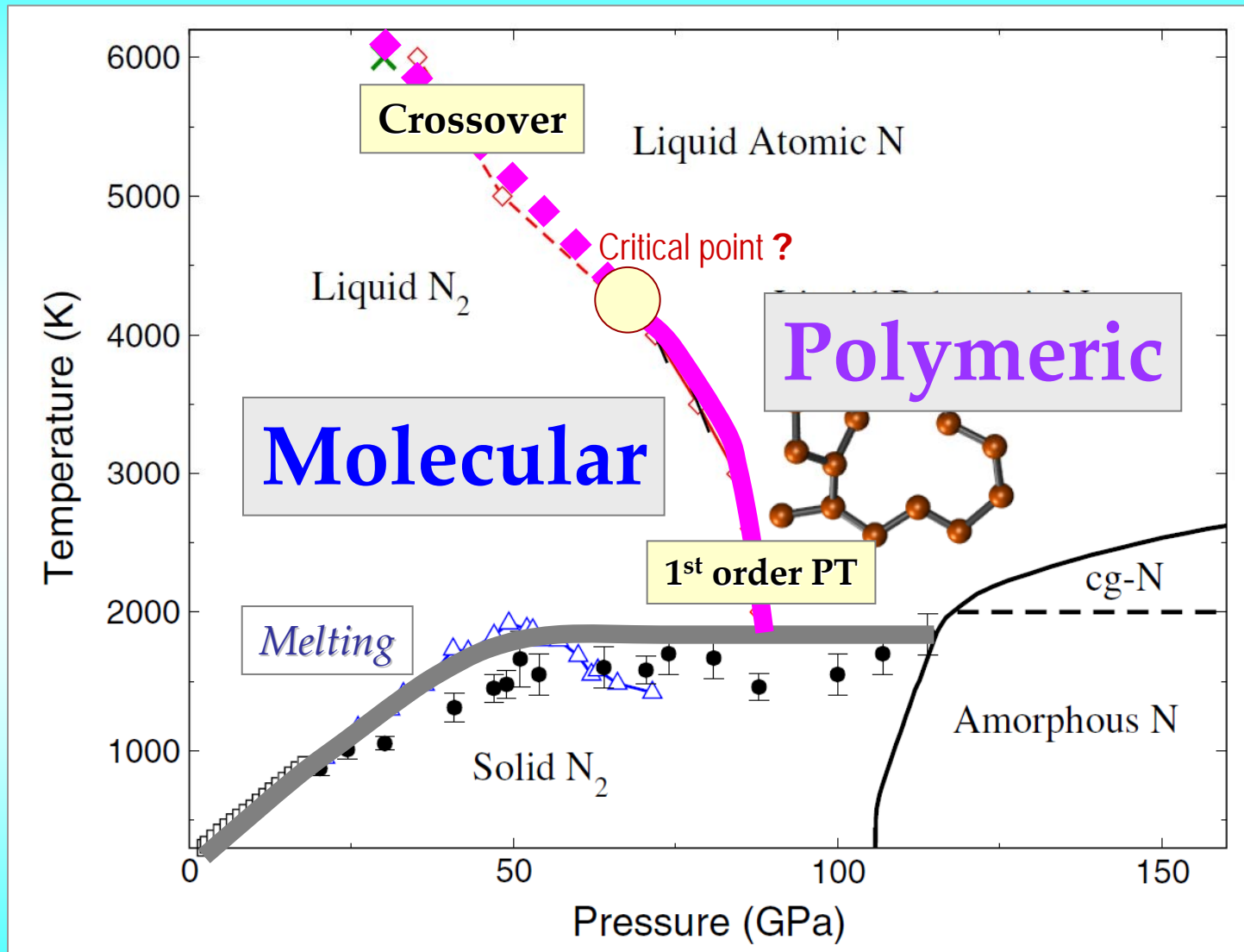
## *First estimations of molecular-polymeric transition*



- 1 - Hugoniot
- 2 - Phase equilibrium line  
Experiment (Nellis et al., 2001)
- 3 - Single shock
- 4 - Double shock

Eugene and Lidia Yakub, *Low Temp. Phys.* **19**, (1993)

# Ab initio calculations - DFT/MD

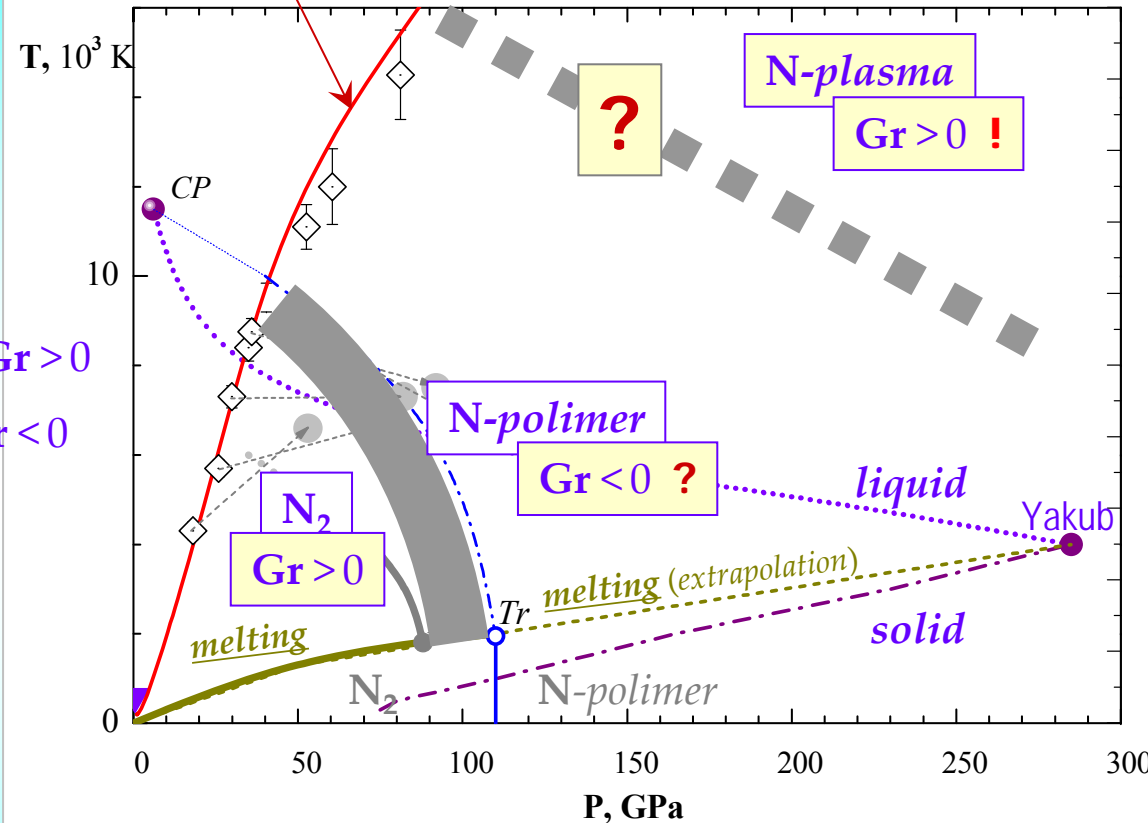


B. Boates, S. Bonev, *Phys. Rev. Lett.*, **102** (2009)

# Nitrogen phase diagram in the region of polymerization

Pressure – temperature

Hugoniot  
Plasma Model (SAHA-code)



**Experiment**

- ◇ – single shock compression, Radousky, Nellis & Ross et al, *Phys. Rev. Lett.* **57** (1986)
- – reflected shock compression, Nellis, Radousky & Hamilton et al, *J. Chem. Phys.* **94** (1991)

**Theoretical models**

- estimation of polymer-molecule boundary in liquid nitrogen (E.Yakub – 1993)
- estimation of polymer-molecule boundary in solid nitrogen (L.Yakub – 1993)
- CP – critical point of 1<sup>st</sup> order phase transition polymer-molecule (E.Yakub – 1993)
- – triple point of 1<sup>st</sup> order phase transition polymer-molecule (E. & L. Yakub – 1993)

E.S. Yakub, / *Low Temp. Phys.* **20** 579 (1994)/  
L.N. Yakub, / *Low Temp. Phys.* **19**, 531 (1993)/

- estimation of polymer-molecule boundary in liquid nitrogen (Ross & Rogers – 2006)

M.Ross & F.Rogers, *Phys. Rev.* **B 74** (2006)

**Ab initio calculations**

- DFT/MD – calculation of of polymer-molecule boundary in liquid nitrogen (S.Bonev et al. – 2009)

- the same as “smoothed” phase transition B. Boates & S. Bonev, *Phys. Rev. Lett.* **102** (2009)

Gr > 0 // Gr < 0 – domains of positive and negative sign of Grüneisen coefficient  $Gr \equiv V(\partial P/\partial E)_V$

hypothetical boundary between polymeric and non-ideal plasma states (1<sup>st</sup>-order phase transition ?)



# Plasma model for nitrogen thermodynamics

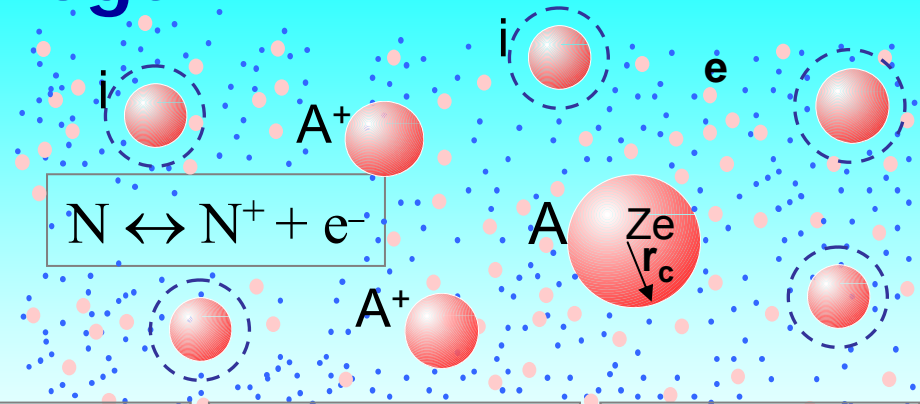
*(code SAHA-N)*

# Shock compression of nitrogen

(chemical picture)

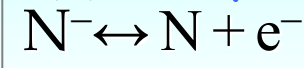
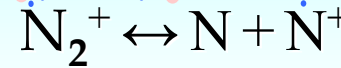
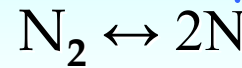
SAHA-code

Gryaznov, Iosilevskiy (1970-2010)



Equilibrium composition:

$\{N_2, N, N^+, e, N_2^+, N^-\}$



Coulomb interaction:

Modified pseudopotential model  
for partially ionized plasma  
(I. Iosilevskiy 1980-2010)

Basic points:

- All assumption are provided at micro-level.
- Input: Choice of  $\Phi_{ie}$ ,  $\Phi_{ii}$  and  $\Phi_{ee}$  pseudopotentials.
- Input: Approximations for binary correlation functions
- Strong correlation of the pseudopotentials for “free” charges and upper energy level for partition functions for bound states.
- Priority for general equalities (*normalizing conditions*) valid independently on degree of non-ideality.
- Non-ideality corrections through the correlation functions and general equalities, valid for Coulomb interaction.

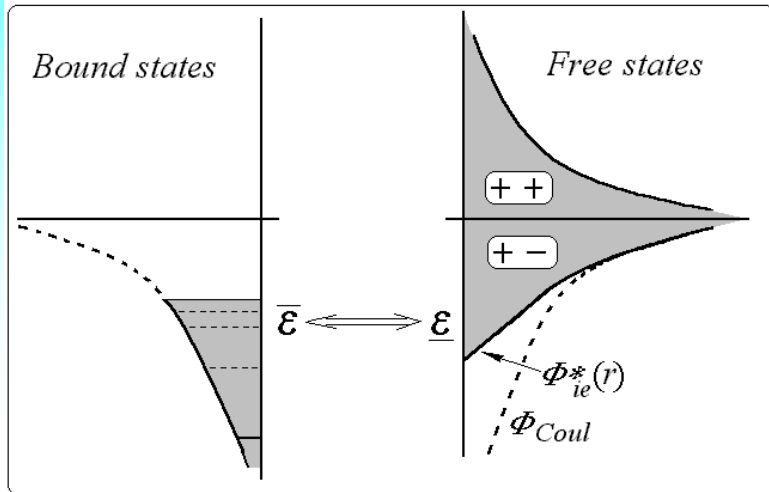
Short range repulsion:

“Soft Spheres” approximation (D. Young)  
modified for *mixture* of soft spheres with  
*different radii* – shift of dissociation level.

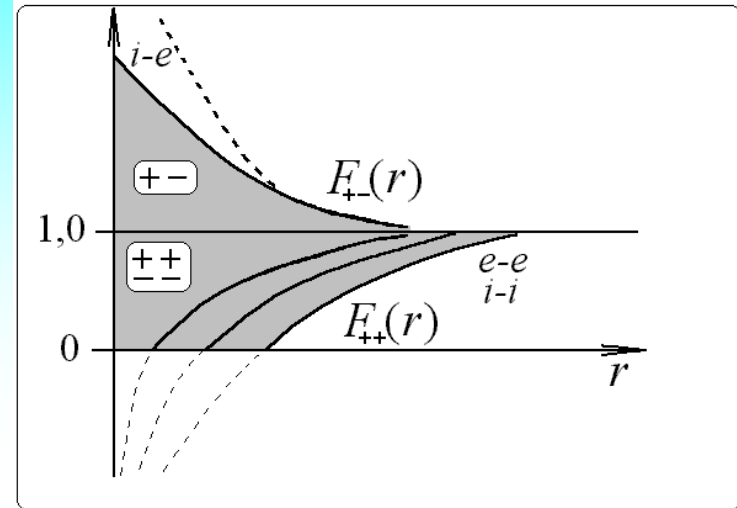
**Key parameter** – ratio of intrinsic volumes: *molecule / atom / ion*:  $R(N)/R(N_2) = 0.63$   
- in accordance with recommendations of “Atom-atomic approximation” of E. Yakub, LT, 1993

# Modified Pseudopotential Approximation (\*):

Bound and free states of electron-ionic pair



Binary *i-i*, *i-e*, *e-e* correlation functions



Effective electro-ionic potential  
(in Glauber's form (1955))

$$\Phi_{ie}^*(r) = -\frac{Z_i e^2}{r} (1 - e^{-r/\sigma}) \geq -\varepsilon$$

↔

The **form** of *i-i*, *i-e*, *e-e* binary correlation functions - «ring» (Debye) approximation with potential  $\Phi_{ie}^*(r)$

$$F_{ab}(r) = 1 \pm A \frac{e^{-pr} - e^{-qr}}{r} \equiv 1 \pm \Psi_0 e^{-vr} \frac{\text{sh}\{\omega r\}}{\omega r}$$

Thermodynamic condition for the depth of *i-e* pseudopotential and amplitude of electron-ionic correlation function

$$-\Psi_0 \approx -\ln F_{ie} \approx \beta [\Phi_{ei}^*(0) - \Delta\mu_e - \Delta\mu_i]$$

"Zero and second moment" conditions (Stillinger & Lovett)

$$n \int [F_+(r) - F_-(r)] dr = 1 \quad n \int [F_+(r) - F_-(r)] \left( \frac{r^2}{r_D^2} \right) dr = 3$$

Positive sign of all correlation functions

↔

$$F_{ab}(r) > 0$$

(\*) Iosilevskiy I. *High Temp.* **18** (1980) // in: "Encyclopedia of Low-T Plasma" (Suppl.), Moscow: FIZMATLIT, 2004, pp. 349

# Thermodynamic contributions in modified pseudopotential model for Coulomb corrections

$$\Phi_{ic}^*(r) = -\frac{Z_i e^2}{r} (1 - e^{-r/\sigma}) \equiv -\left(\frac{Z_i e^2}{\sigma}\right) \frac{(1 - e^{-r/\sigma})}{r/\sigma} \geq -\Phi_{ic}^*(0) \sim -\varepsilon$$

Pseudopotentials



$$F_{ab}(r) = 1 \pm A \frac{e^{-pr} - e^{qr}}{r} \equiv 1 \pm \Psi_0 e^{-vr} \frac{sh \omega r}{\omega r}$$

Correlation Functions

Homogeneity of Coulomb potential  $\Leftrightarrow$

$$U = U_{Kin} + U_{Pot} \quad 3PV = 2U_{Kin} + U_{Pot}$$

Total Energy correction

$$\Delta U = -Vn^2 \int (F_+ \Phi_{ei}^* - F_- \Phi_{ii}^*) d\mathbf{r}$$

Potential Energy Correction -  $\Delta U_{Pot}$

$$\Delta U_{pot} = -Vn \int \Phi_{coul} (F_+ - F_-) d\mathbf{r}$$

Pressure Correction -  $\Delta P$

$$3\Delta PV = (2\Delta U - \Delta U_{pot}) = (2\Delta U_{kin} + \Delta U_{pot})$$

Approximate relation between Coulomb corrections for chemical potential and energy ( $\Delta\mu \Leftrightarrow \Delta U/N$ )

$$\Delta\mu_i = \Delta\mu_e \approx (N_i + N_e)^{-1} \Delta U$$

**NB !**

*Positive shift in average kinetic energy due to non-ideality of free charges subsystem*

$$\Delta U_{kin} = 3\Delta PV - \Delta U$$

Well-known relation between pressure and energy corrections for *free charges subsystem*

$$\Delta U = 3\Delta PV$$

which is valid at weak non-ideality ( $\Gamma \ll 1$ ), is **no longer valid** in strong non-ideality conditions ( $\Gamma \sim 1$ )

It is equivalent to **additional effective electron-ion repulsion**

(in comparison with ordinary one-parametric Coulomb corrections, depending on non-ideality parameter only

$$\Delta F/NkT = f(\Gamma)$$

**Experimental data  $\Leftrightarrow$  Theoretical models**

*(comparison)*

## Summary

# Thermodynamics of shock compressed nitrogen (primary thermodynamic results of experiment)

**High-temperature part of Hugoniot is close to isochore**

$$\rho \approx 3.3 \pm 0.1 \text{ g/cc} \quad (90 < P < 330 \text{ GPa})$$

Internal energy is almost linear on pressure at isochore

$$\text{Gr} = V(\partial P/\partial E)_V \approx \text{const} \approx 0.62$$

Temperature is almost linear on pressure at isochore

$$(\partial p/\partial T)_V \approx \text{const} \approx 4.54 \text{ (GPa/K)}$$

$$Z \equiv PV/RT \equiv P/n_N kT \approx \text{const} \approx 2.66 \pm 0.20$$

Internal energy is almost linear on temperature at isochore

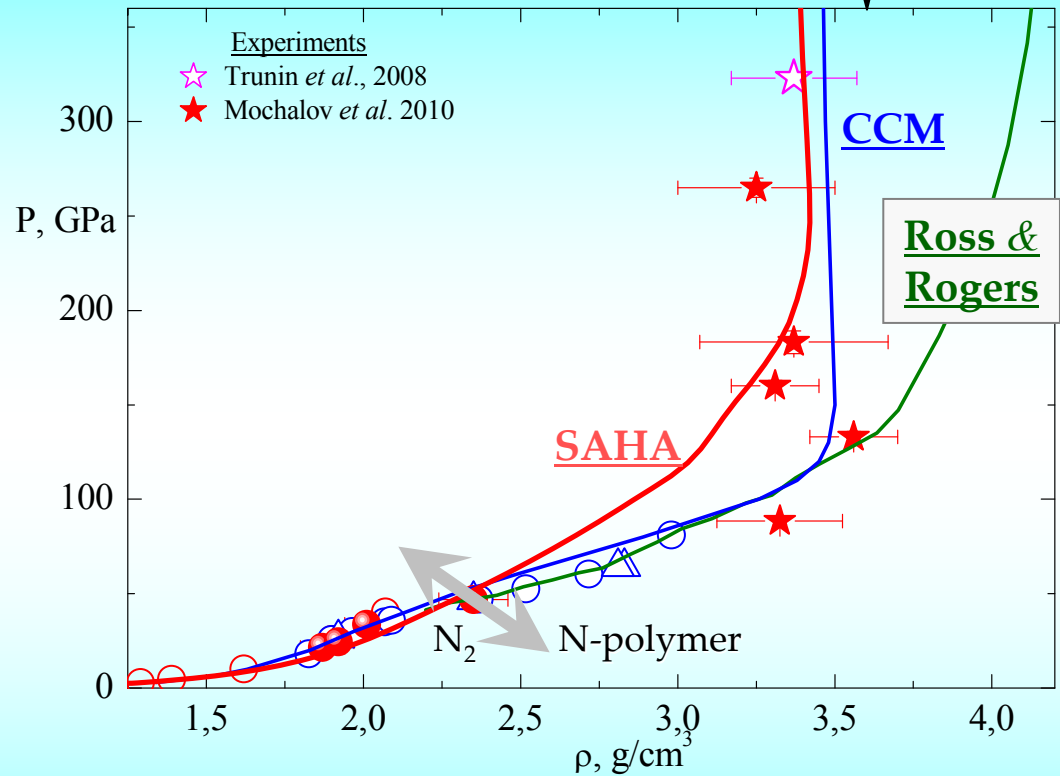
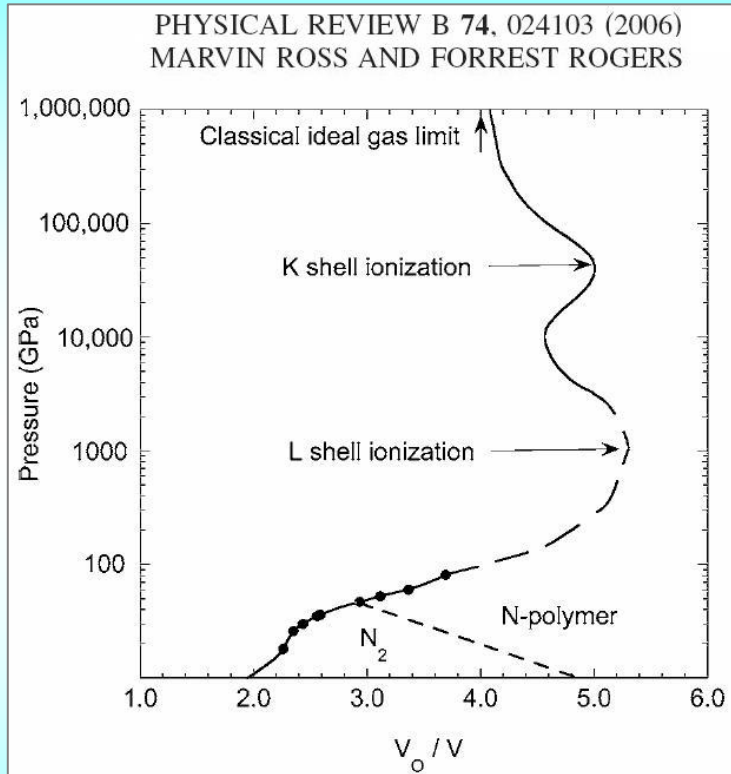
$$C_V \equiv (\partial E/\partial T)_V \approx \text{const} \approx 2.06 \text{ (J/g}\cdot\text{K)}$$

# Check of theoretical models

## Quasi-isochoric behavior of nitrogen Hugoniot

$$90 < P_{\text{Hug}} < 330 \text{ GPa}$$

$$\rho_{\text{Hug}} \approx 3.3 \pm 0.1 \text{ g/cm}^3$$

 $\sigma_{\text{lim}}$ 


SAHA-code (V. Gryaznov & I. Iosilevskiy)

CCM – Compressible Covolume Model  
(A. Medvedev & V. Kopyshv)

★ - Mochalov M., Zhernokletov M. et al.,  
*JETP*, 137 (2010)

☆ - Trunin R., Boriskov G., et al.  
*JETP Letters*, 88 (2008)

## Summary

# Thermodynamics of shock compressed nitrogen (primary thermodynamic results of experiment)

High-temperature *part of Hugoniot is close to isochore*

$$\rho \approx 3.3 \pm 0.1 \text{ g/cc} \quad (90 < P < 330 \text{ GPa})$$

**Internal energy** *is almost linear function of pressure at isochore*

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Temperature is almost linear on pressure at isochore

$$(\partial p/\partial T)_V \approx \text{const} \approx 4.54 \text{ (GPa/K)}$$

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**Internal energy** is almost linear on temperature at isochore

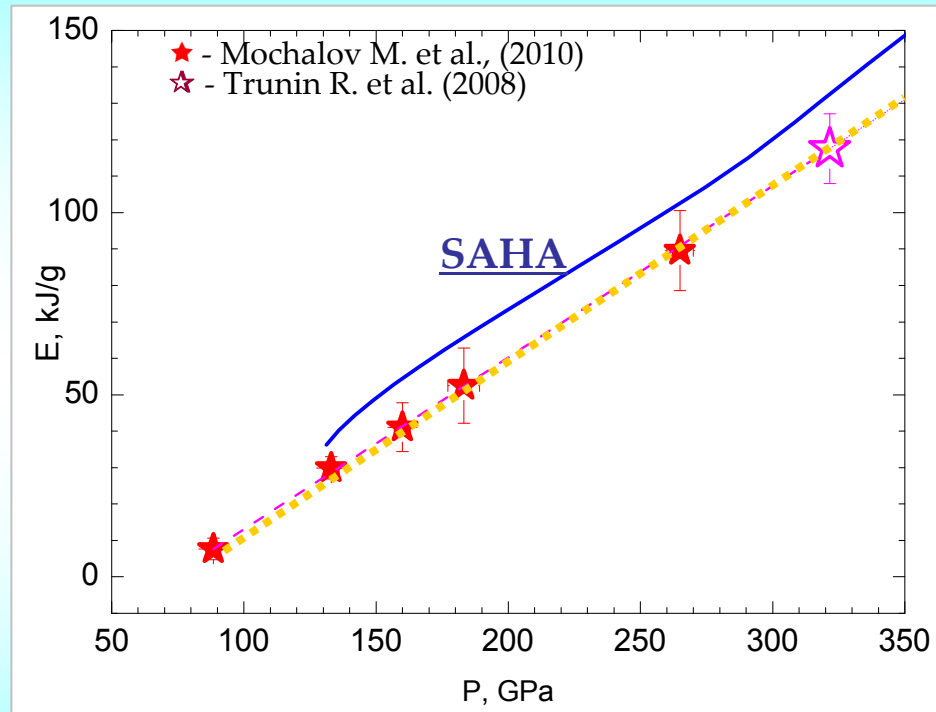
$$C_V \equiv (\partial E/\partial T)_V \approx \text{const} \approx 2.06 \text{ (J/g}\cdot\text{K)}$$



# Quasi-linear behavior of $E(p)$ at $\rho = \text{const}$

*Hugoniot*:  $\sim \rho \approx \text{const}$  ( $3.3 \pm 0.1$  g/cc)

Internal Energy  $\Leftrightarrow$  Pressure (*Hugoniot*)



$\rho \approx 3.3 \pm 0.1$  g/cc  
 $90 < P < 330$  GPa

Blue curve – internal energy calculated via plasma model  
(code SAHA / Gryaznov, Iosilevskiy)

NB ! (\*) Reference point – energy of ideal atomic gas N at  $T = 0$  K



$$\text{Gr} = V(\partial P / \partial E)_V \approx \text{const} \approx 0.62$$

## Summary

# Thermodynamics of shock compressed nitrogen (primary thermodynamic results of experiment)

High-temperature part nitrogen Hugoniot is close to be isochoric

$$\rho \approx 3.3 \pm 0.1 \text{ g/cc} \quad (90 < P < 330 \text{ GPa})$$

Internal energy is almost linear on pressure at isochore

$$\text{Gr} = V(\partial P/\partial E)_V \approx \text{const} \approx 0.62$$

Temperature is almost linear on pressure at isochore

$$(\partial p/\partial T)_V \approx \text{const} \approx 4.54 \text{ (GPa/K)}$$

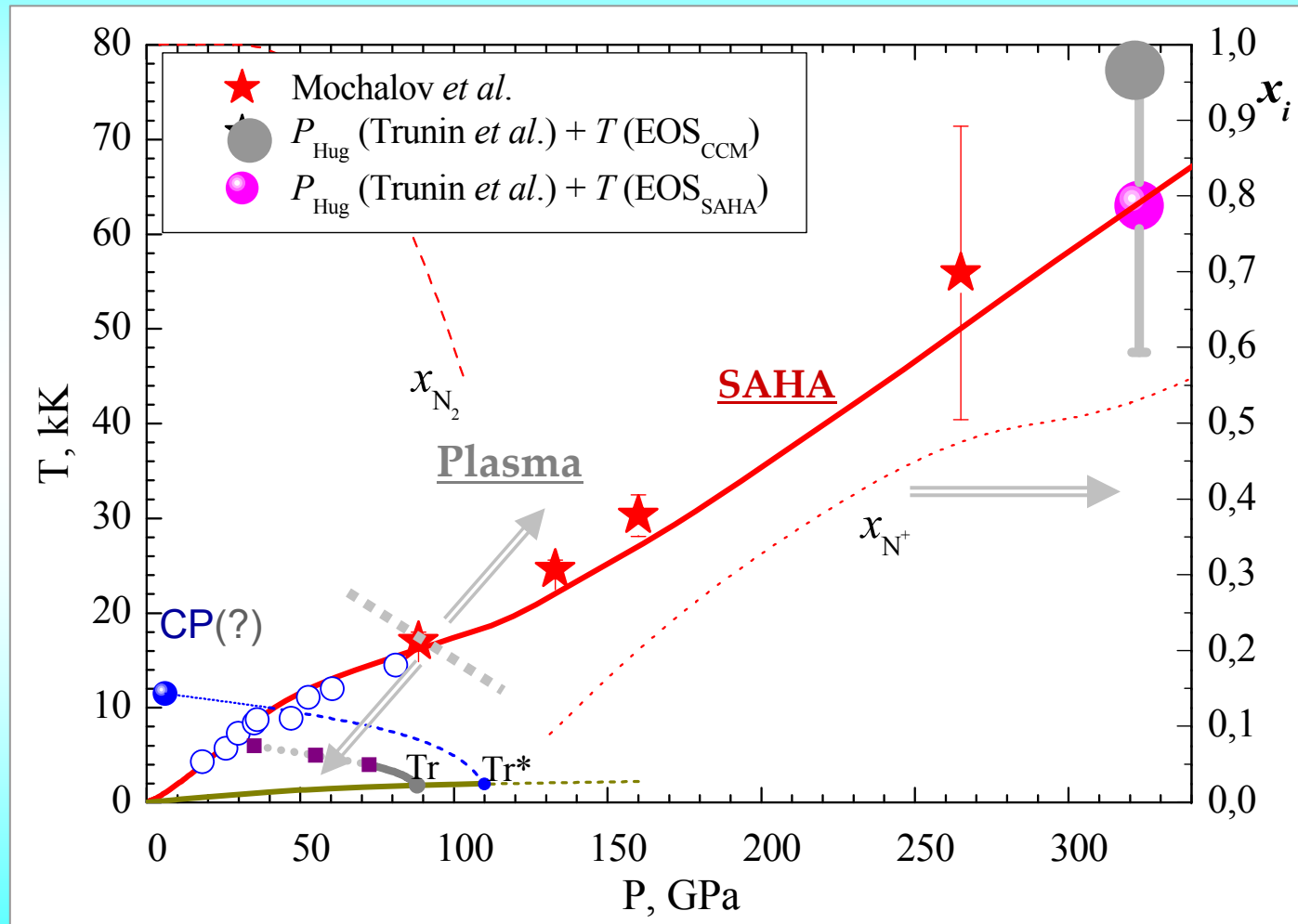
$$Z \equiv PV/RT \equiv P/n_N kT \approx \text{const} \approx 2.66 \pm 0.20$$

Internal energy is almost linear on temperature at isochore

$$C_V \equiv (\partial E/\partial T)_V \approx \text{const} \approx 2.06 \text{ (J/g}\cdot\text{K)}$$

# Temperature of shock compressed nitrogen

## General $P$ - $T$ diagram

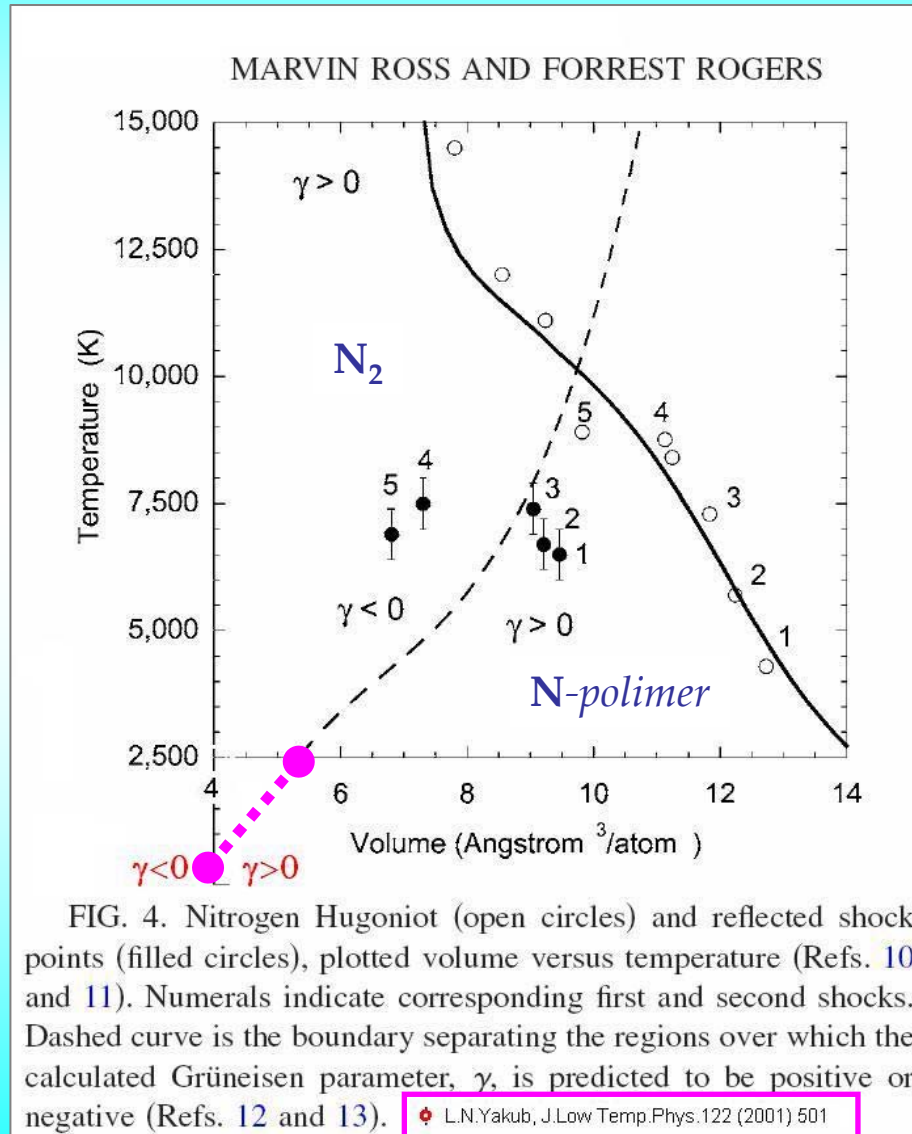


Quasi-linear behavior of  $T(p)$  at  $q = const$



# Positive and negative Grüneisen coefficient

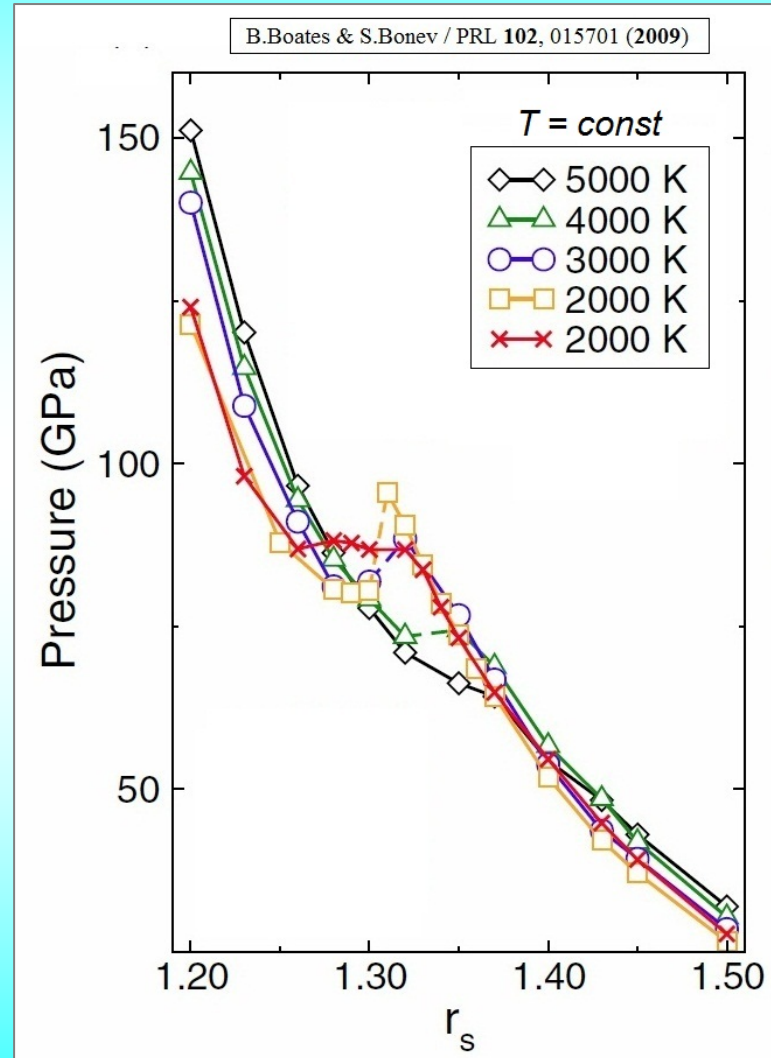
$$\gamma \equiv \text{Gr} \equiv V(\partial P/\partial E)_V$$



**Anomalous thermodynamics** *with* **Gr < 0**  
*how it looks like for?*

# Anomalous thermodynamics *with $Gr < 0$*

*how it looks like for?*



# Conclusions *and* perspectives

- **New experimental** data on **shock compression** of cryogenic liquid **nitrogen** in megabar pressure range "**open new page**" in investigation of properties for warm dense matter of "simple" molecular gases
- **New experimental** data in nitrogen may be considered as the thermodynamic manifestation of **non-standard** form of **pressure ionization** (*from polymeric to plasma state*)
- This new form of **pressure ionization** (*from polymeric to plasma state*) seems to be **general, universal** and **interesting** phenomenon
- **Simultaneous** measurements of **caloric** and **thermal** equation of state (EOS) (*pressure, density, temperature and internal energy*) along Hugoniot give powerful tool for **checking** theoretical **models** and "calibration" of wide-range EOS-s
- It is **promising** to continue and extend **experimental** investigation of **pressure ionization** of **polymeric** state via intense HIB and laser heating
- It is **promising** to study **pressure ionization** of **polymeric** state in **direct numerical simulations** ("numerical experiment") DFT\_MD, PIMC, WP\_MD...*etc*



# Perspectives

## *Modelling*

### Improvement of Plasma model (*SAHA-code*):

- *From EOS of soft spheres to EOS of {exp - 6} potential system*

### Improvement of Polymeric models (*E. & L. Yakub*):

- *Calibration of both model on results of ab initio calculations (DFT/MD)*

### Collaboration (*Gryaznov, Iosilevskiy ⇔ E. & L. Yakub*)

- *Incorporation of polymeric state model into SAHA-code*

New approaches are desirable: (*new calculations and comparisons*)

- *Ab initio*: RPIMC, DPIMC // DFT/MD // WPMD // TBM . . .
- *Wigner-Zeits cell model*: TFC, MHFS, . . .
- . . . . .
- *Semiempirical (wide-range) EOS-s*
- . . . . .

# Perspectives

*(new experiments)*

- ! - Strong **shock compression** of **liquid** nitrogen at high pressure ( $P > 3$  Mbar)
- ! - Strong **shock compression** of **solid** nitrogen at high pressure ( $P > 3$  Mbar)
- ! - Strong **shock compression** of **pre-compressed gaseous** nitrogen at high pressure (*measurement of series of Hugoniot with varying initial densities (like in VNIIEF experiments with deuterium)*)
- ! - Strong **isentropic compression** of nitrogen by explosive at Mb pressure *search of density discontinuity (hypothetical phase transition ?) on nitrogen isentrope(s) (like in VNIIEF's experiments with deuterium (M.Mochalov, V.Fortov et al. PRL, 2007))*

## Exotics:

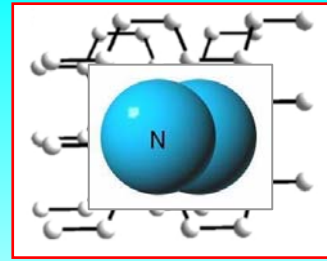
- ! - Heavy Ion Beam *and* Laser heating of cryogenic nitrogen
- .....



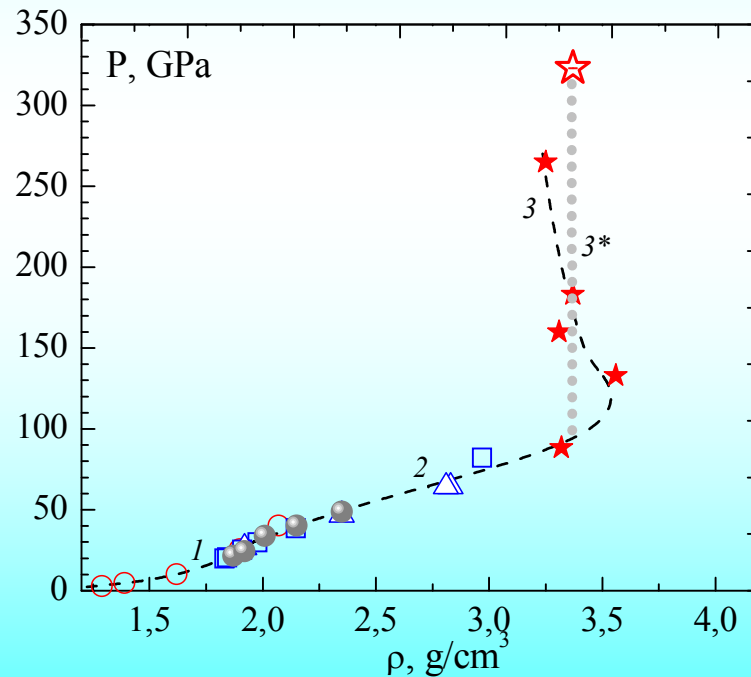
# Plasma Physics with Intense Heavy Ion and Laser Beams

*GSI, Darmstadt, Germany*

May 2 - 4, 2011



# Thank you!



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