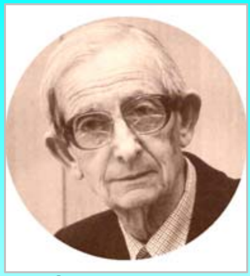


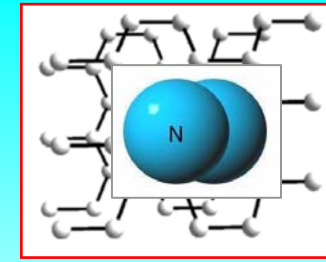
Sarov, 2011

Annual Moscow Workshop

Non-ideal Plasma Physics

Russian Academy of Science

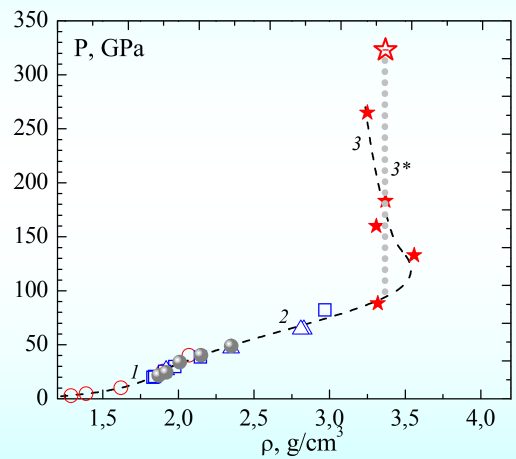
November 23-24, 2011



Chernogolovka, 2010
EMMI_GSI, 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

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

IPCP RAS

MIPT

Shock compression of liquid nitrogen

(new experimental data in megabar pressure 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*

Russian Federal VNIIEF Nuclear Center

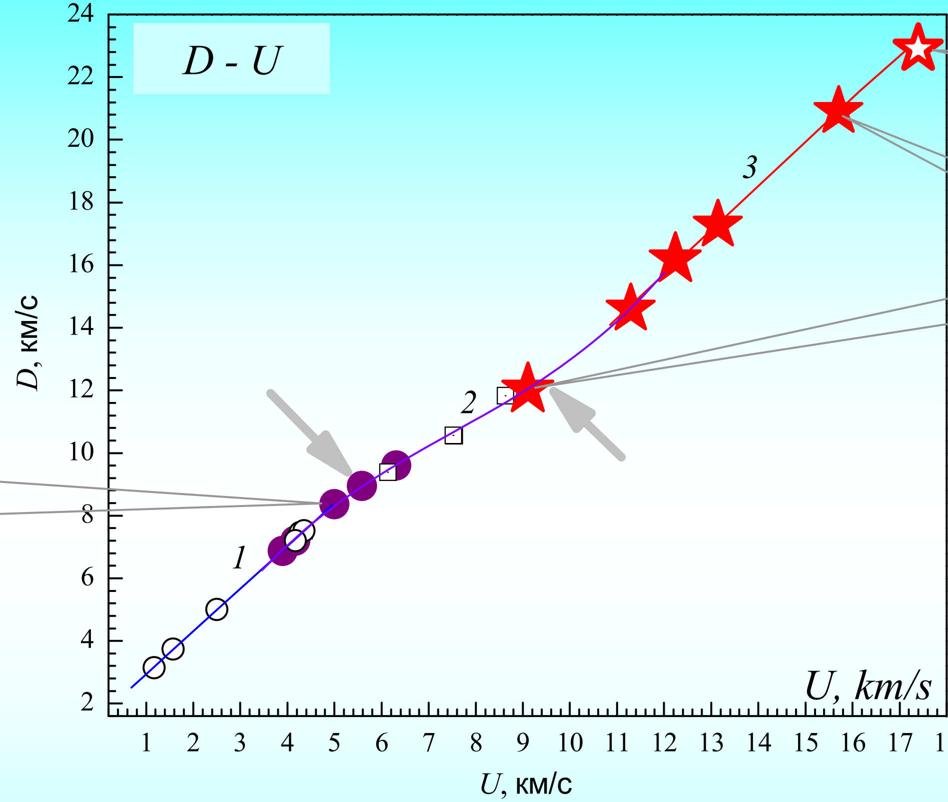
Collaboration:

Eugene & Lidia Yakyb

(Odessa University, Ukraine)

Shock Hugoniot of liquid nitrogen

(primary experimental data in kinematic variables)



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

D and U – shock and mass velocities

Arrows – hypothetical transitions between molecular (*1*), polymeric (*2*) and plasma (*3*) states

Initial state

$\rho_0 = 0.81$

($T_0 = 77$ K)

Approximations (Mochalov et al.2010):

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)

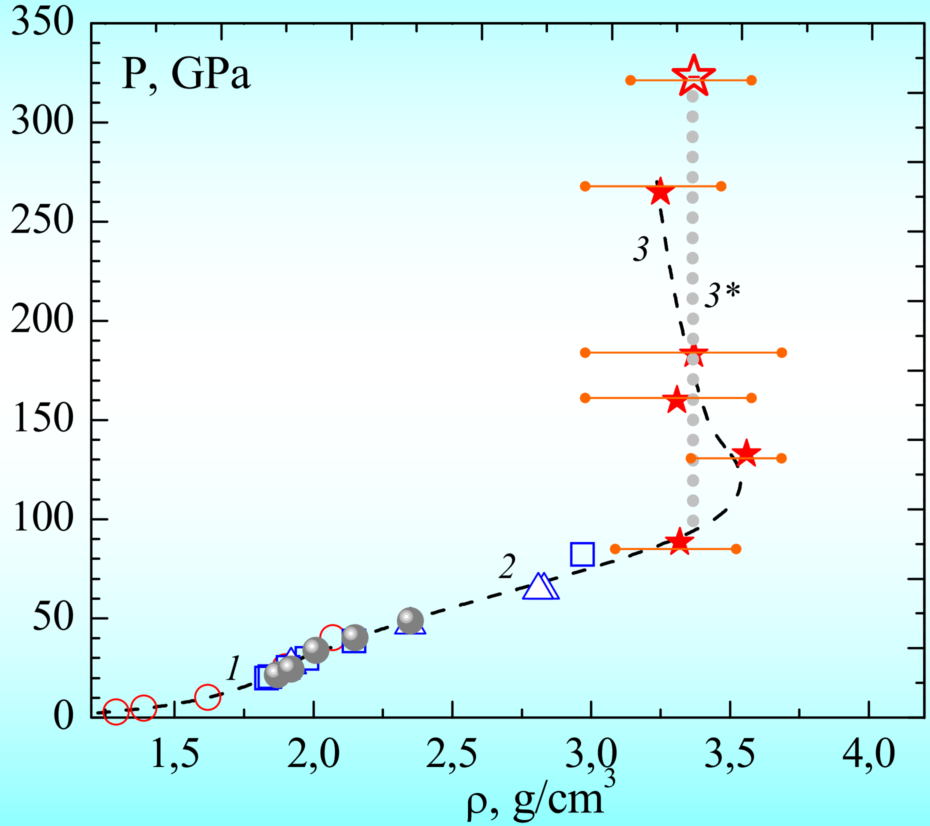
Shock Hugoniot of liquid nitrogen

(experimental data in thermodynamic variables)

$$p_1 = p_0 + \rho_0 DU$$

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

$$\rho_1 = \rho_0\{D/(D-U)\}$$



P, GPa	**ρ**, g/cm³	ρ/ρ_0
88.4 ± 2	3.325 ± 0.2	**4.12**
133.3 ± 3	3.56 ± 0.15	**4.41**
160.0 ± 3	3.31 ± 0.25	**4.10**
183.0 ± 3	3.37 ± 0.35	**4.18**
265.0 ± 5	3.25 ± 0.25	**4.03**
323	3.37 ± 0.20	**4.16**

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

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

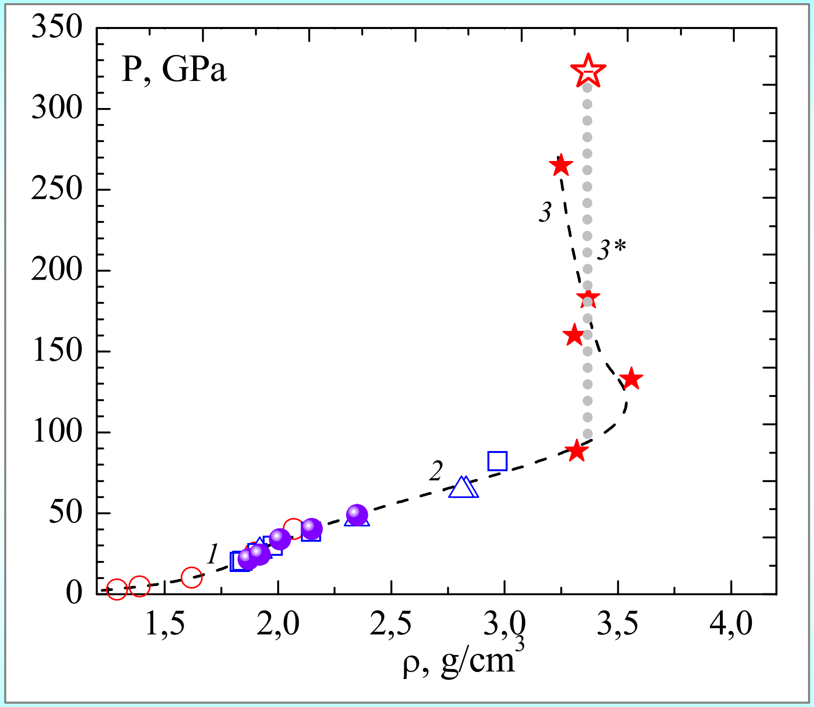
☆ - Trunin R., Boriskov G., Bykov A., Medvedev A. *JETP Letters*, **88**, 220 (**2008**)

Internal energy is close to be linear function of pressure!

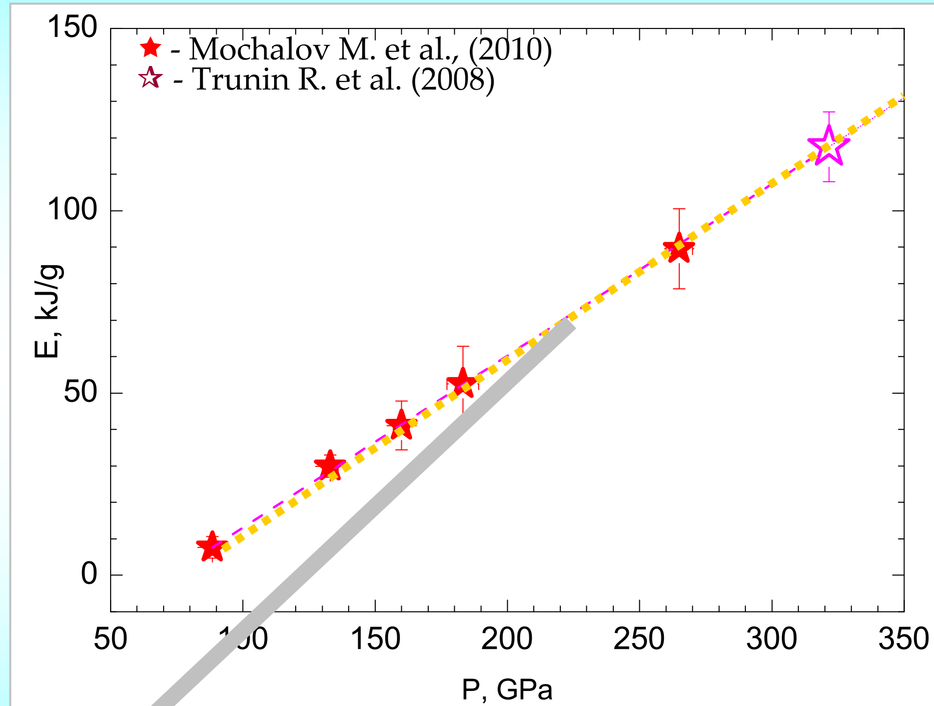
$$E_1 = E_0 + \frac{1}{2}\left(\frac{1}{\rho_0} - \frac{1}{\rho_1}\right)(p_1 + p_0)$$

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

Hugoniot: $\sim \rho \approx const$ (3.3 ± 0.1 g/cc)



Internal Energy ⇔ Pressure of sock compressed nitrogen



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

NB !

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

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

What does it mean ?

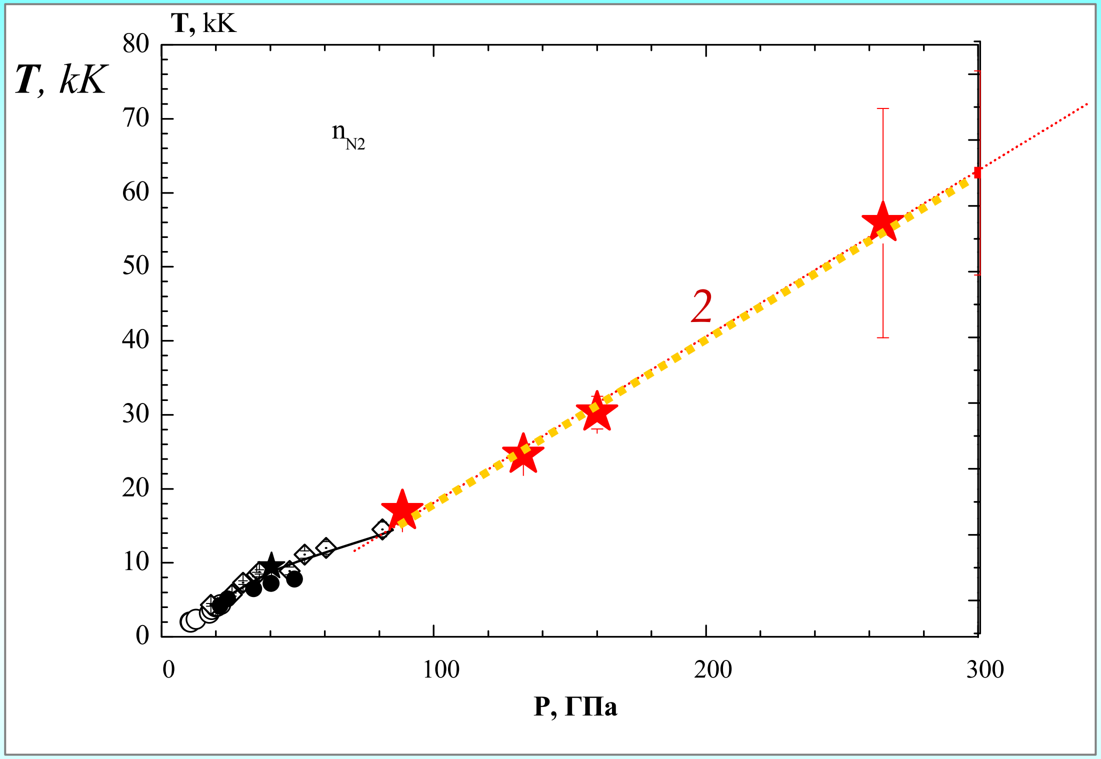
The region of approximate constancy for Gruneizen parameter ⇔ $\rho \approx 3.3 \pm 0.1$ g/cc $90 < P < 330$ GPa

Temperature of shock compressed nitrogen

measurements of thermal equation of state

P, GPa	***T*, kK**
88.4 ± 2	**16**.2 ± 0.9
133.3 ± 3	**24**.6 ± 0.5
160.0 ± 3	**28**.4 ± 2.2
183.0 ± 3	-
265.0 ± 5	**56**.0 ± 15.2
323	**-**

JETF **137**, 77 (20**10**)

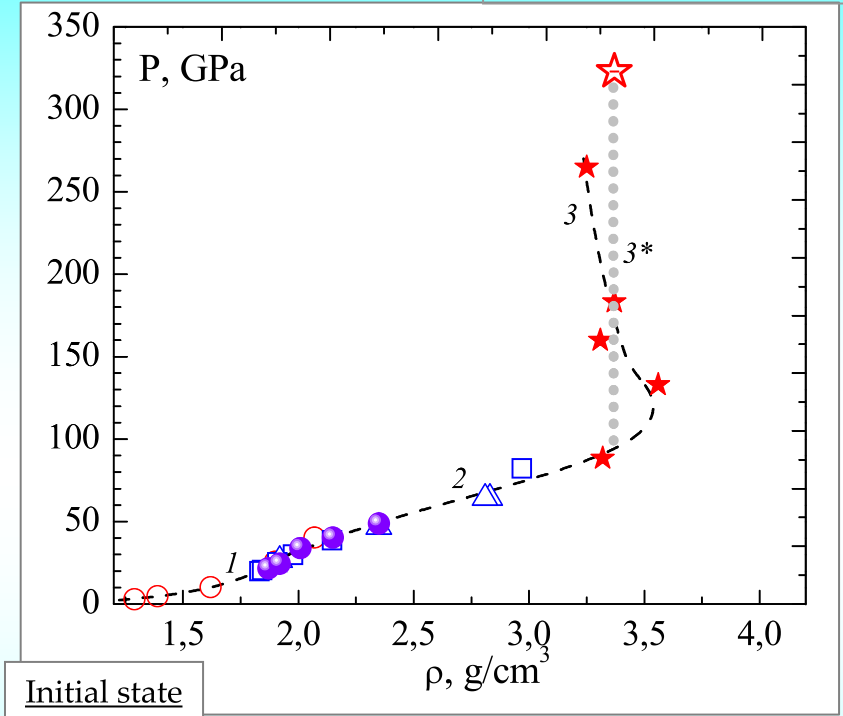


- Experiment (Mochalov M., Zhernokletov M. et al., *JETF* **137**, 77 (20**10**)

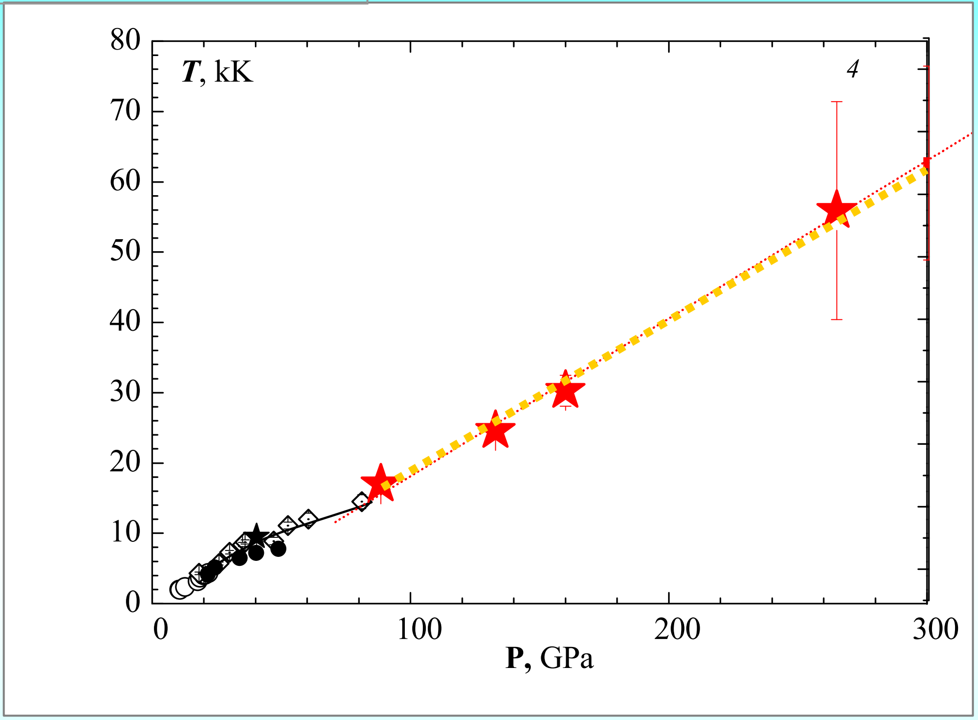
2 – linear approximation of experimental data (*P* ≈ 90 – 300 ГПа)

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

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



Initial state
$\rho_0 = 0.81$



★ - Mochalov et al., *JETP* (2010)

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

NB !

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

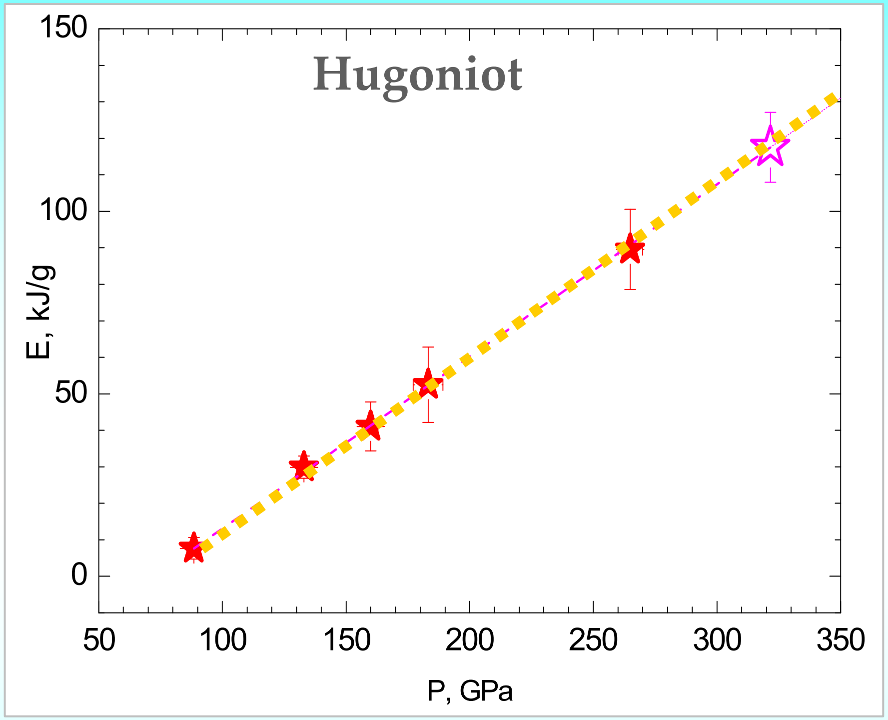
PV/RT

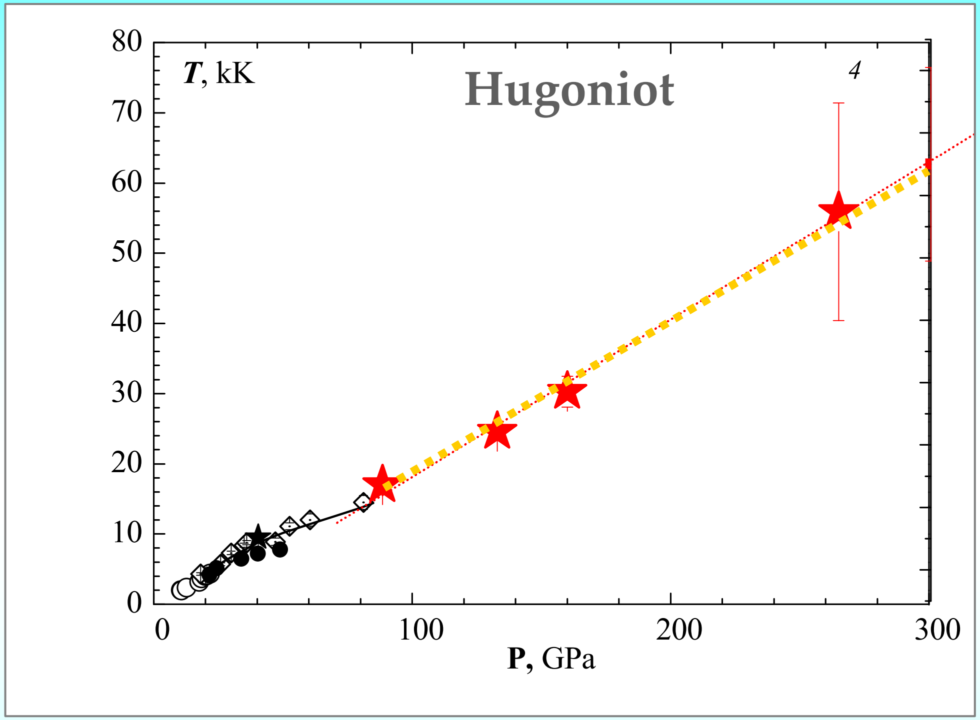
Ideal gas N_2: Z= **0.5**
Ideal gas N: Z= **1.0**
Id. gas N^+ + e: Z= **2.0**
……

What does it mean ?

Internal energy ~ linear function on temperature at isochore

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





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

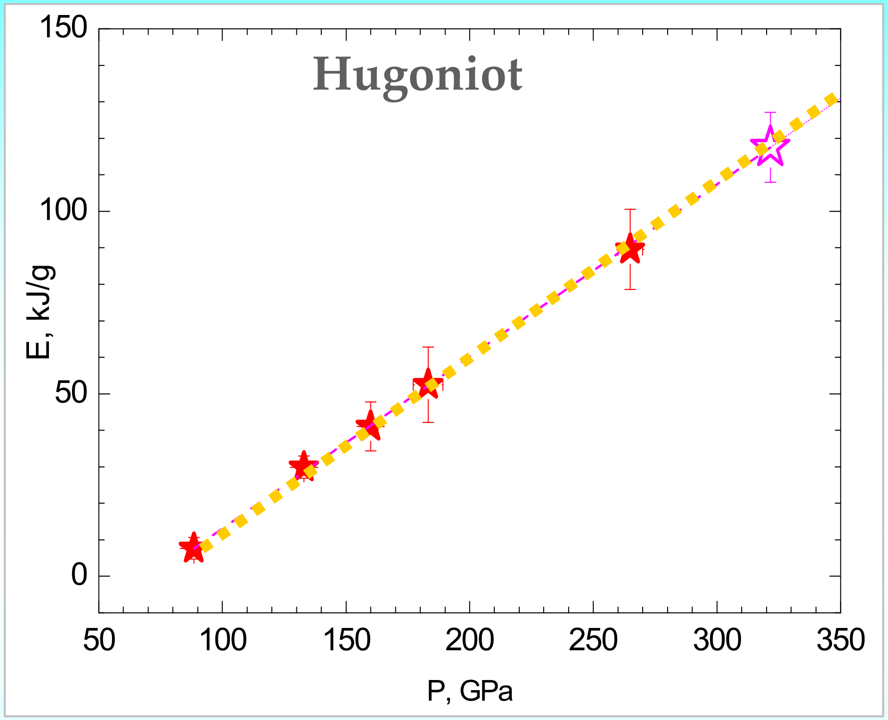
NB ! $C_v \equiv (\partial E/\partial T)_v \approx const \approx 2.0$ (J/gK)

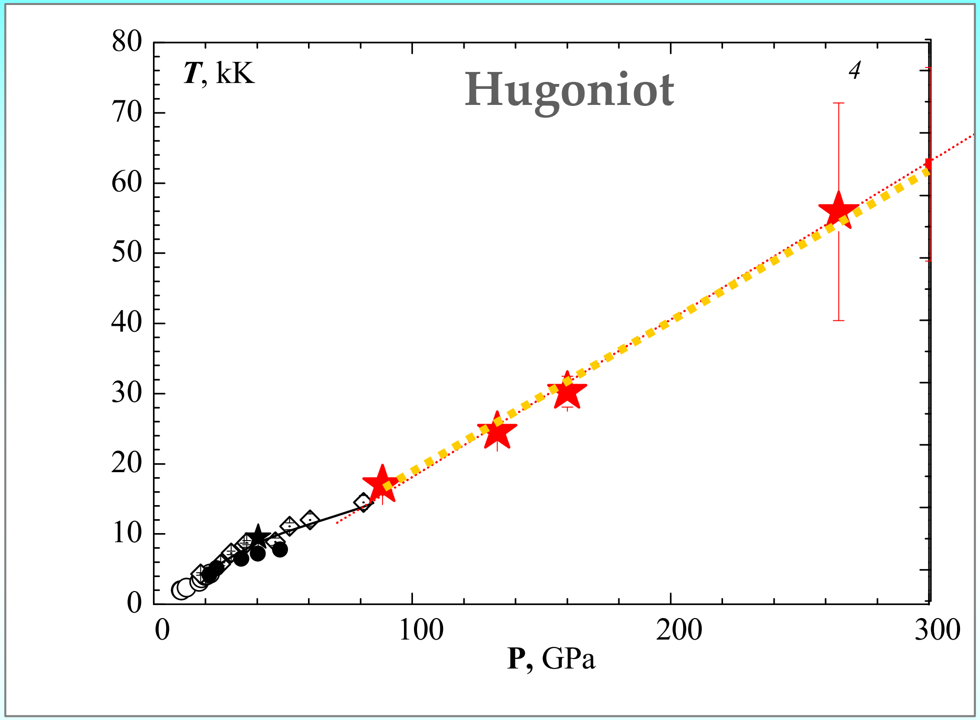
$C_V/R_N \approx 3.5$ **!**

What does it mean ?

Constancy *of* **Grüneizen parameter** *and* **Heat capacity** *at isochore*

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





Gr $\approx$ ***const*** **+ $C_V \approx$ *const*** ⇔ **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

High-temperature part nitrogen Hugoniot is close to be isochoric

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

Internal energy is almost linear on pressure at isochore

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

Temperature is almost linear on pressure at isochore

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

$$Z \equiv PV/RT \equiv P/n_{\mathrm{N}}kT \approx const \approx 2.66 \pm 0.20$$

Internal energy is almost linear on temperature at isochore

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

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

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

Expected behavior of nitrogen Hugoniot

M.Ross & F.Rogers

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

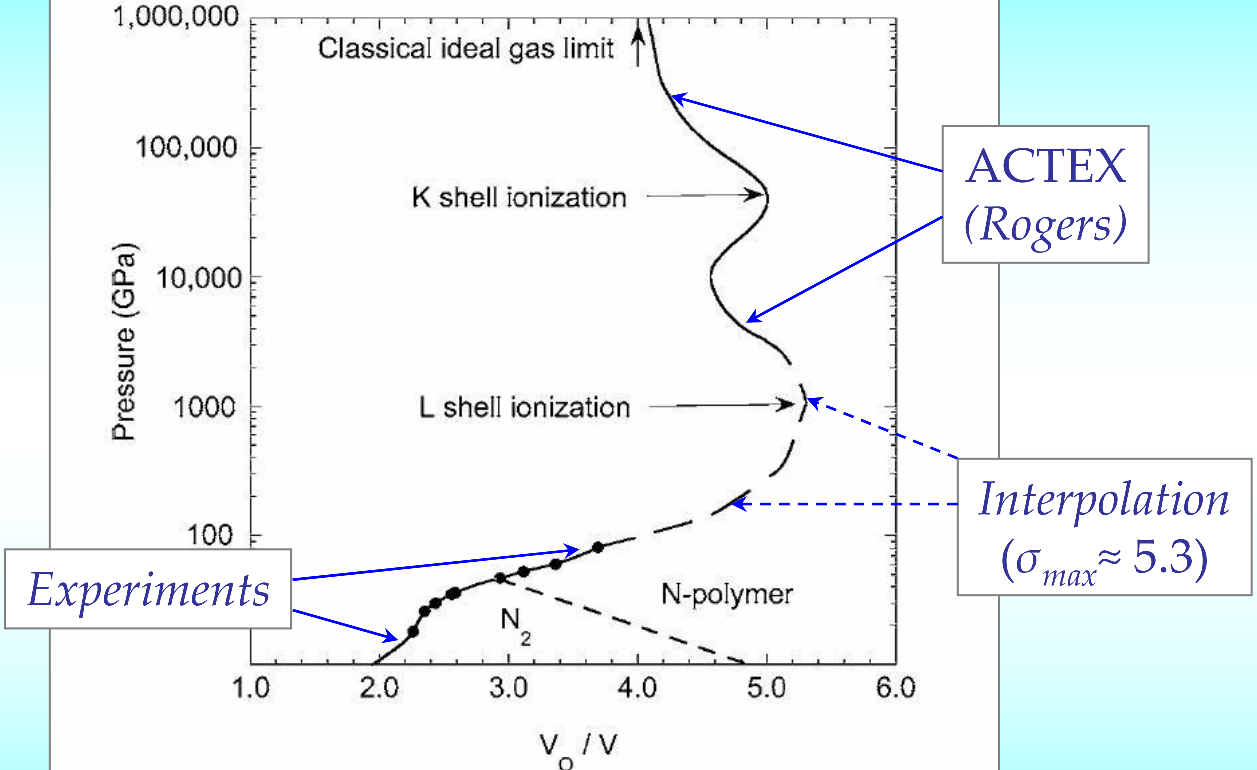
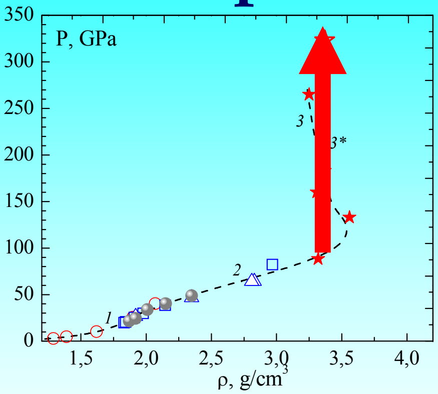


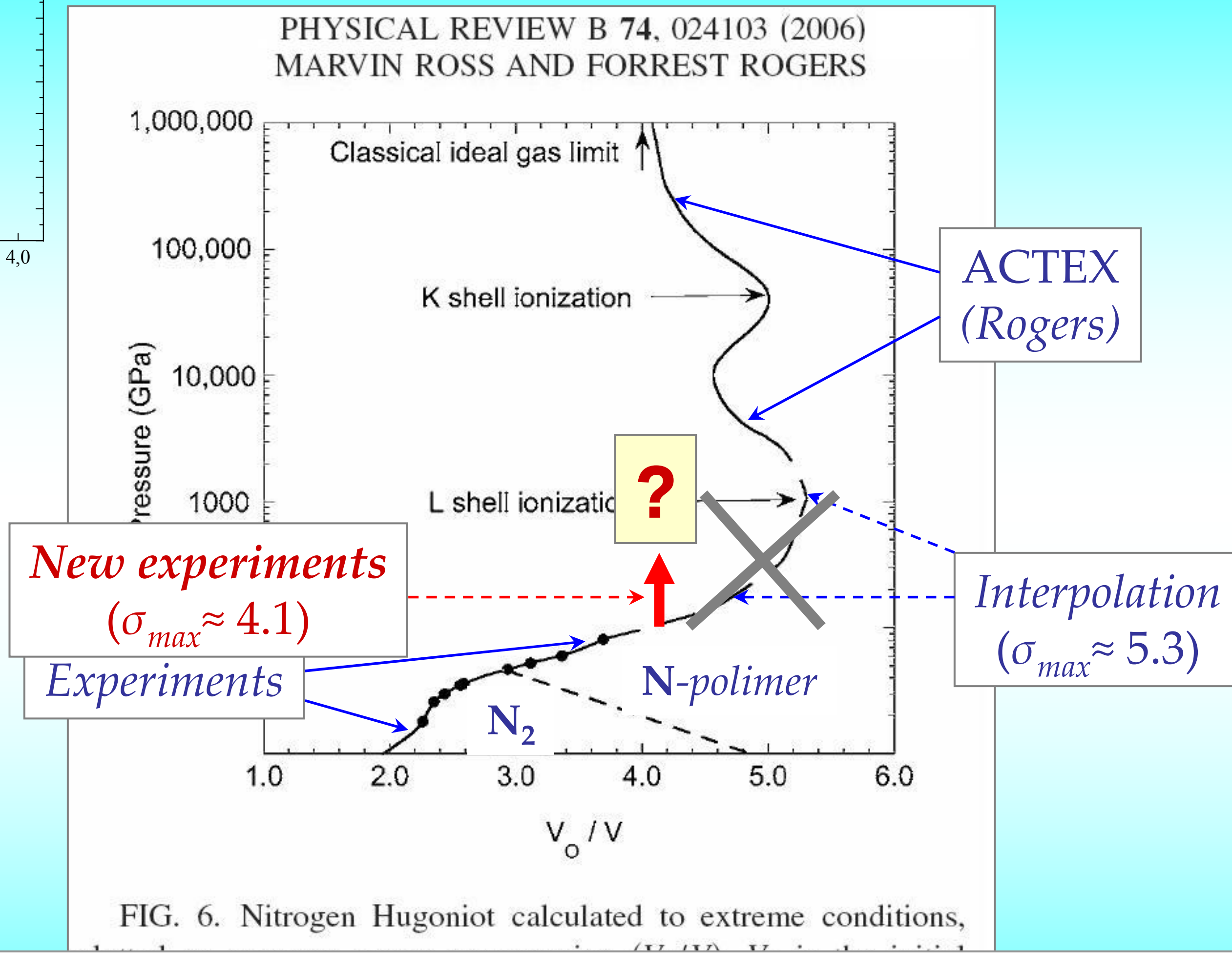
FIG. 6. Nitrogen Hugoniot calculated to extreme conditions, plotted as pressure versus compression (V_0/V). V_0 is the initial liquid volume. Experimental data (filled circles) (Ref. 11), connected to ACTEX calculations (solid curve) by a smoothed interpolation (long-dashed curve). The small dashed line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

New experiments *vs* expected behavior *of* nitrogen Hugoniot



M.Ross & F.Rogers

???



NB !

New experiments *are* **in strong contradiction**
with **expected behavior** *of* **nitrogen Hugoniot**

Nitrogen Hugoniot problem in plasma state – what do we need?

New experiments ?
- Shock waves
- Isentropic Compression
- Heavy Ion Beams
- Laser Heating

. . . . . *etc. etc.*

Theory ?

Ab initio

RPIMC, DPIMC

DFT/MD WP/MD

Chemical models

SAHA-S

SAHA-N

(Gryaznov *et al.*)

WZ-cell models

TF, TFC, MHFS…

. . . . . .

Wide-range EOS-s

IPCP RAS

JIHT RAS

CCM (*Sarov*)

. . . . . .

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

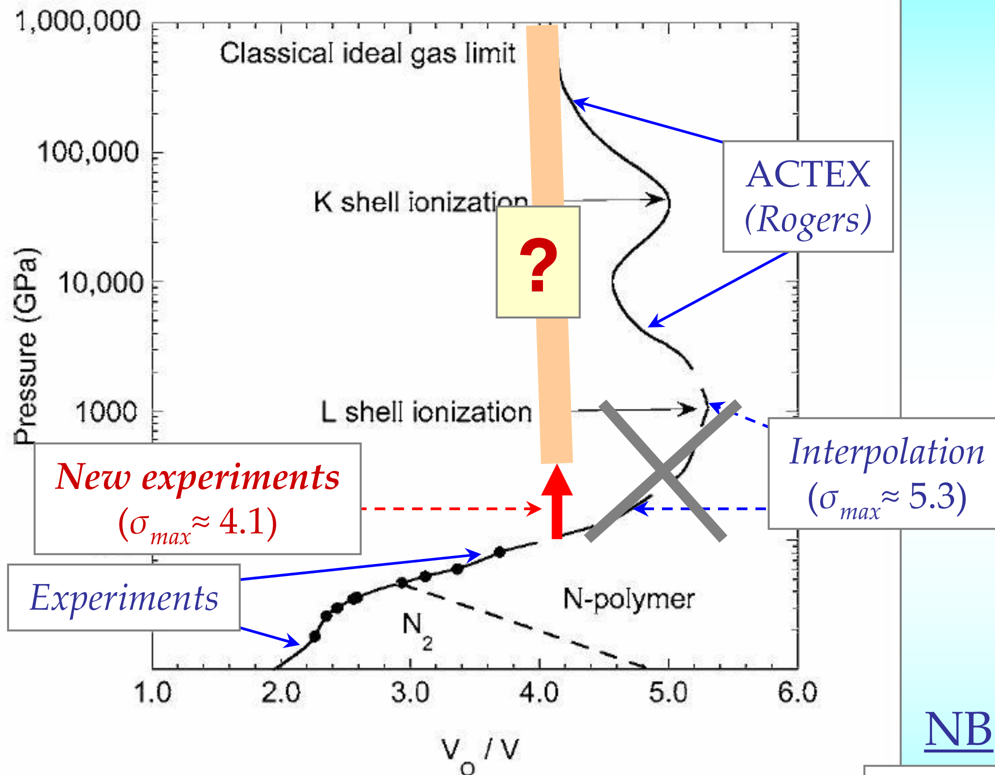


FIG. 6. Nitrogen Hugoniot calculated to extreme conditions plotted as pressure versus compression (V_0/V). V_0 is the initia[l] liquid volume. Experimental data (filled circles) (Ref. 11), con[-]nected to ACTEX calculations (solid curve) by a smoothed interpo[-]lation (long-dashed curve). The small dashed line locates approxi[-]mately the liquid molecular-polymer transition.

NB !

In last experiments on deuterium compression:

$P_{max} \approx$ **50** Mbar

(see: Mochalov et al. NPP-2011)

(Mochalov et al. JETP Lett. 2010)

Nitrogen Hugoniot

(comes trough polymeric phase ?)

New experiments ?
- Shock waves
- Heavy Ion Beams
- Laser Heating

. . . . . etc. etc.

THEORY ?

Ab initio

RPIMC, DPIMC

DFT/MD, WP/MD..

Chem. models

SAHA-S

SAHA-N

. . . . . .

WZ-cell models

TFC, MHFS, . . .

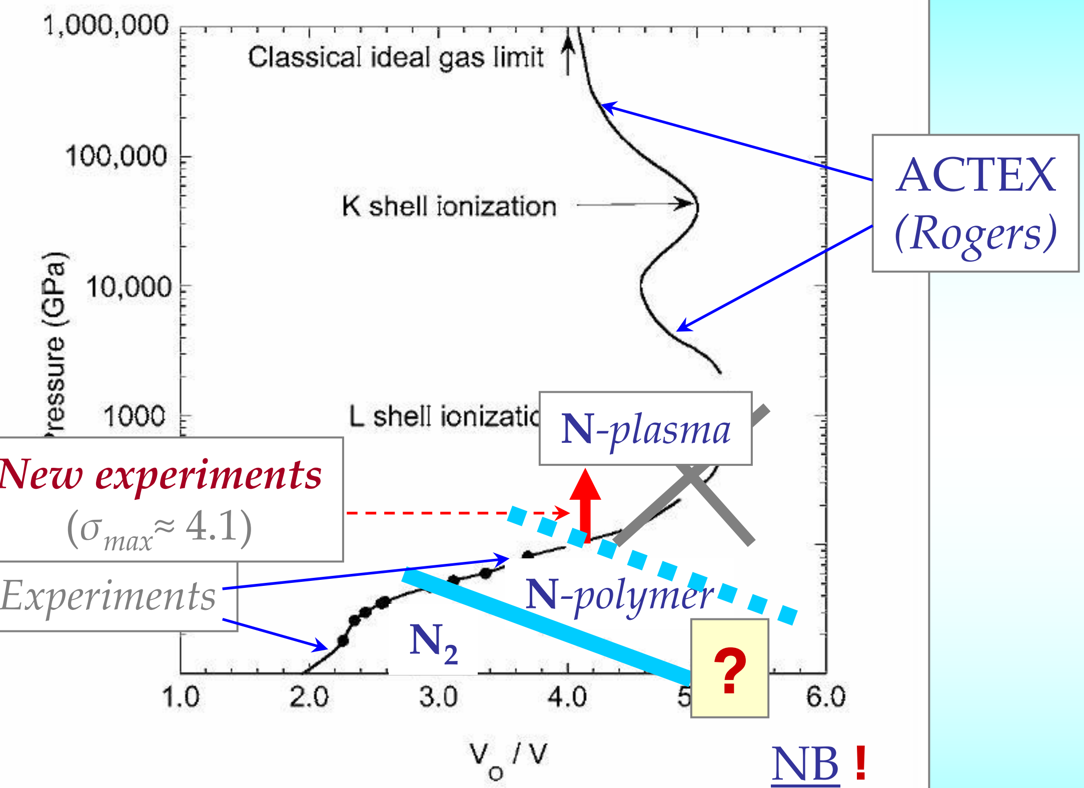
. . . . . .

Wide-range EOS

CCM (*Sarov*)

. . . . . .

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



NB !

FIG. 6. Nitrogen Hugoniot calculate
plotted as pressure versus compression
liquid volume. Experimental data (filled
nected to ACTEX calculations (solid curv
lation (long-dashed curve). The small das
mately the liquid molecular-polymer trans

Polymeric state
is expected between
molecular and plasma
regions
(see below)

Ab initio calculations - DFT/MD

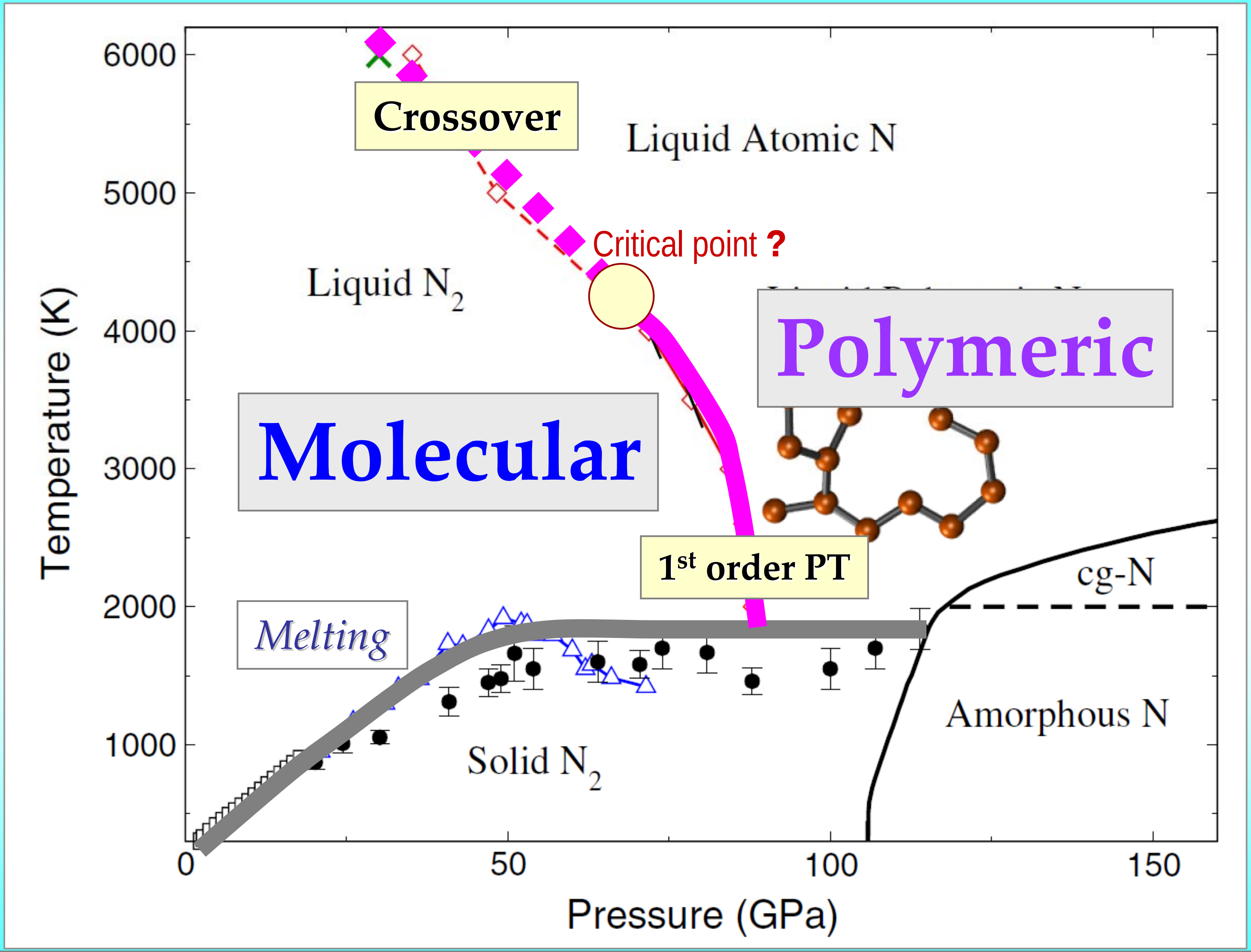


figure from
B. Boates, S. Bonev, *Phys. Rev. Lett.*, **102** (2009)

Ab initio calculations - DFT/MD

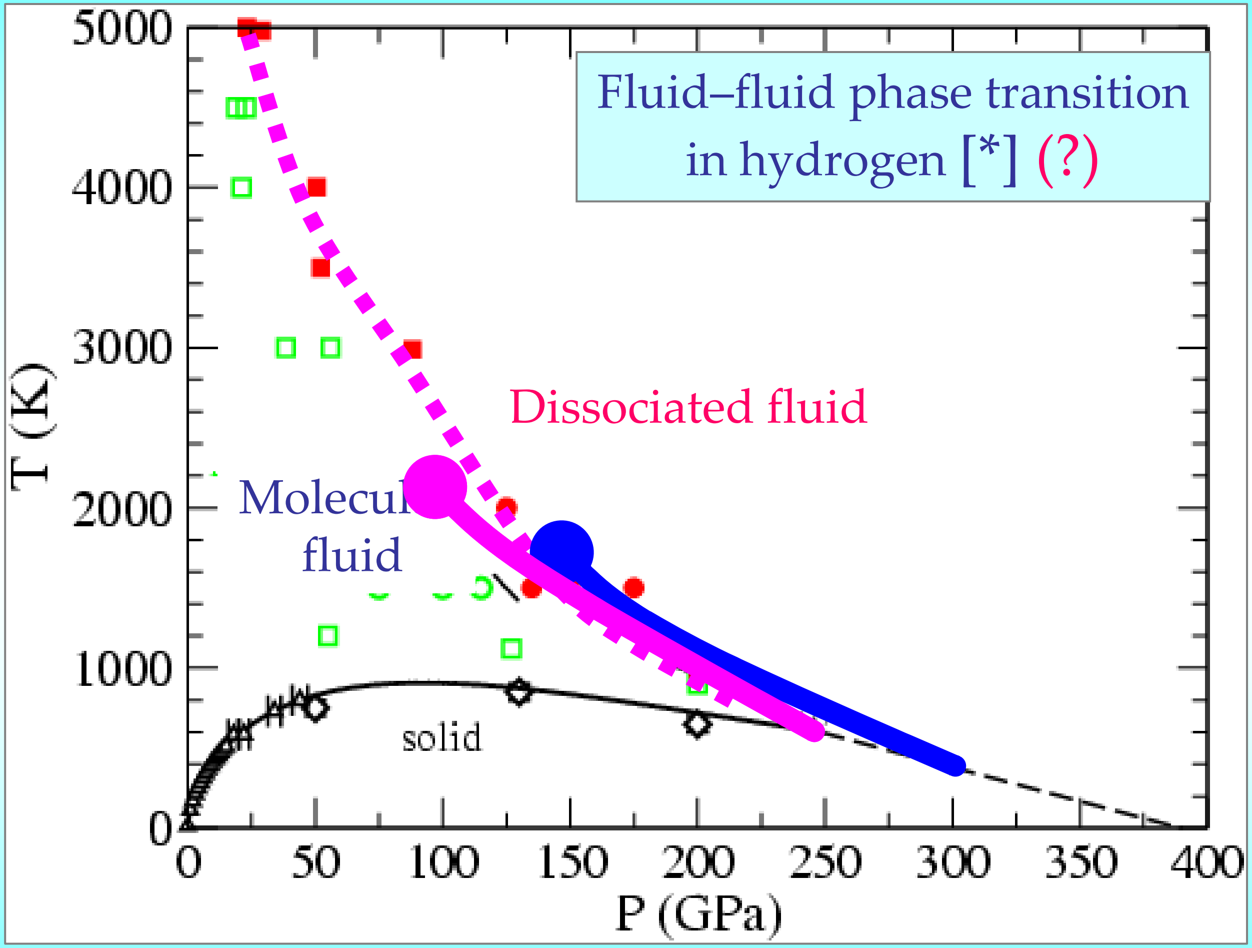


Figure from:
Giulia Galli,
SCCS-2005,
Moscow
= = @ = =
with additions:
Morales et al. *2010*
and
Lorensen et al. *2010*

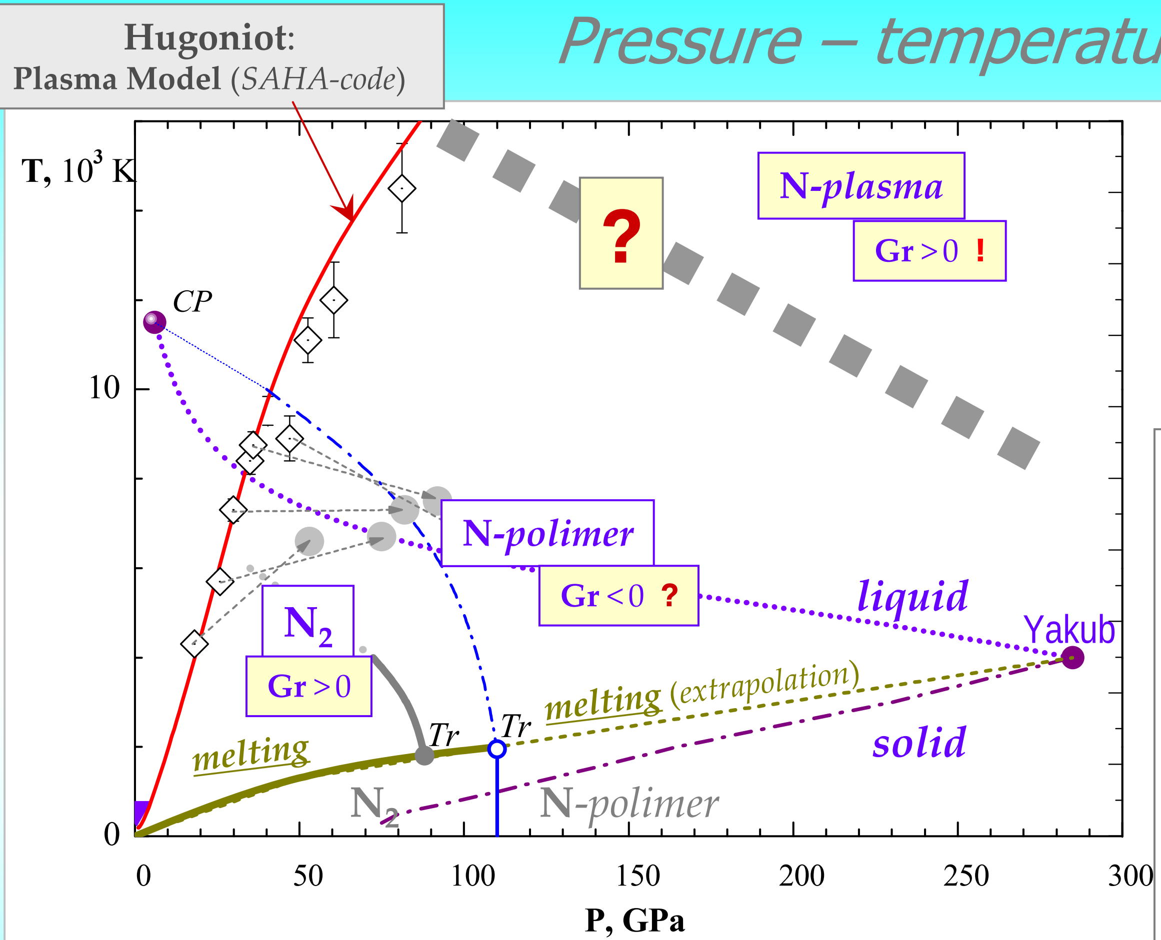
Morales *et al*, 2010

Lorenzen *et al*, 2010

DFT/MD: Scandolo S. *PNAS* **100**, (2003) // Bonev S., Militzer B., Galli G. *PRB* **69** (2004)
WPMD : Jakob B. *et al. PRE* (2007) // **DFT/MD**: Morales M. *et al. PNAS* **107**, (2010)/
DFT/MD: Lorenzen W. *et al. PRB* (2010)

Nitrogen phase diagram in the region of polymerization

Pressure – temperature



Experiment

◇ – single shock compression,
● – reflected shock compression
Radousky, Nellis & Ross et al, *Phys. Rev. Lett.* **57** (1986)
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 1st order phase transition polymer-molecule (E.Yakub – 1993)

● – triple point of 1st 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 (1st-order phase transition or continuous **?**)

Phase Diagram of Dense Nitrogen

(*summary*)

New experiments ?
- Shock waves
- Iso-*S* Compression
- Heavy Ion Beams
- Laser Heating

. . . . . *etc. etc.*

THEORY ?

Ab initio

RPIMC, DPIMC

DFT/MD

Chem. models

SAHA-N

. . . . . .

WZ-cell models

TFC, MHFS, . . .

. . . . . .

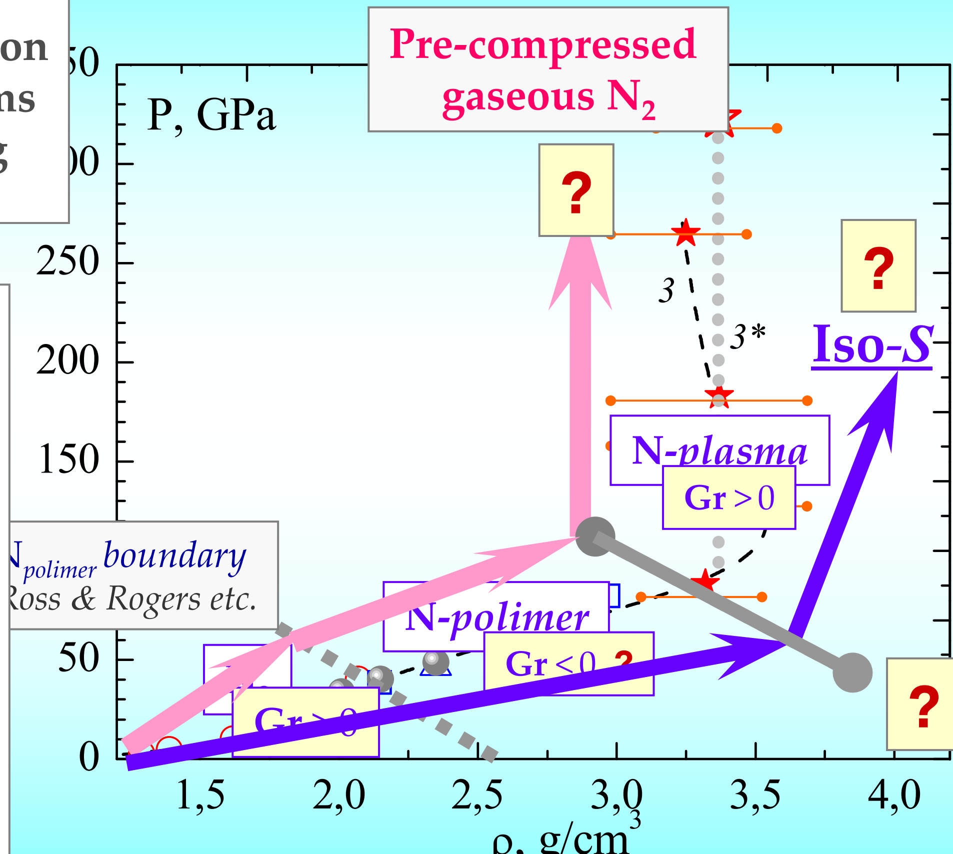
Wide-range EOS

EOS (*IPCP RAS*)

EOS (*JIHT RAS*)

CCM (*Sarov*)

. . . . . .



Hypothetical Pressure Ionization
from N-polymer
to
N-plasma

1st-order phase transition ?

Critical point(s) ?

Domain: Gr < 0 ?

Topology of the boundary: Gr = 0 ?

? ? ? ? ?

★ - Mochalov M., Zhernokletov M. et al., *JETP* **137**, 77 (**2010**) // ☆ - Trunin R., Boriskov G., Bykov A., Medvedev A. *JETP Letters*, **88**, 220 (**2008**)

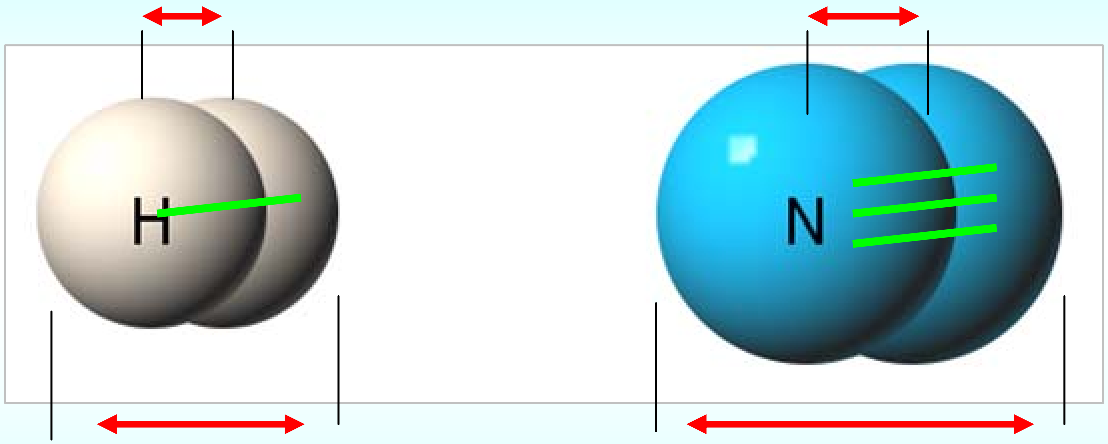
Comments

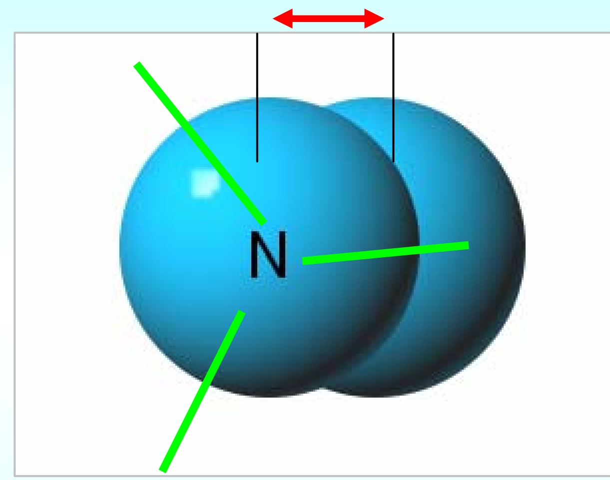
microphysics

Simple molecules: $H_2 \Leftrightarrow N_2$

Triple covalent bond

D_e= 9.8 eV (4.9 eV/atom)





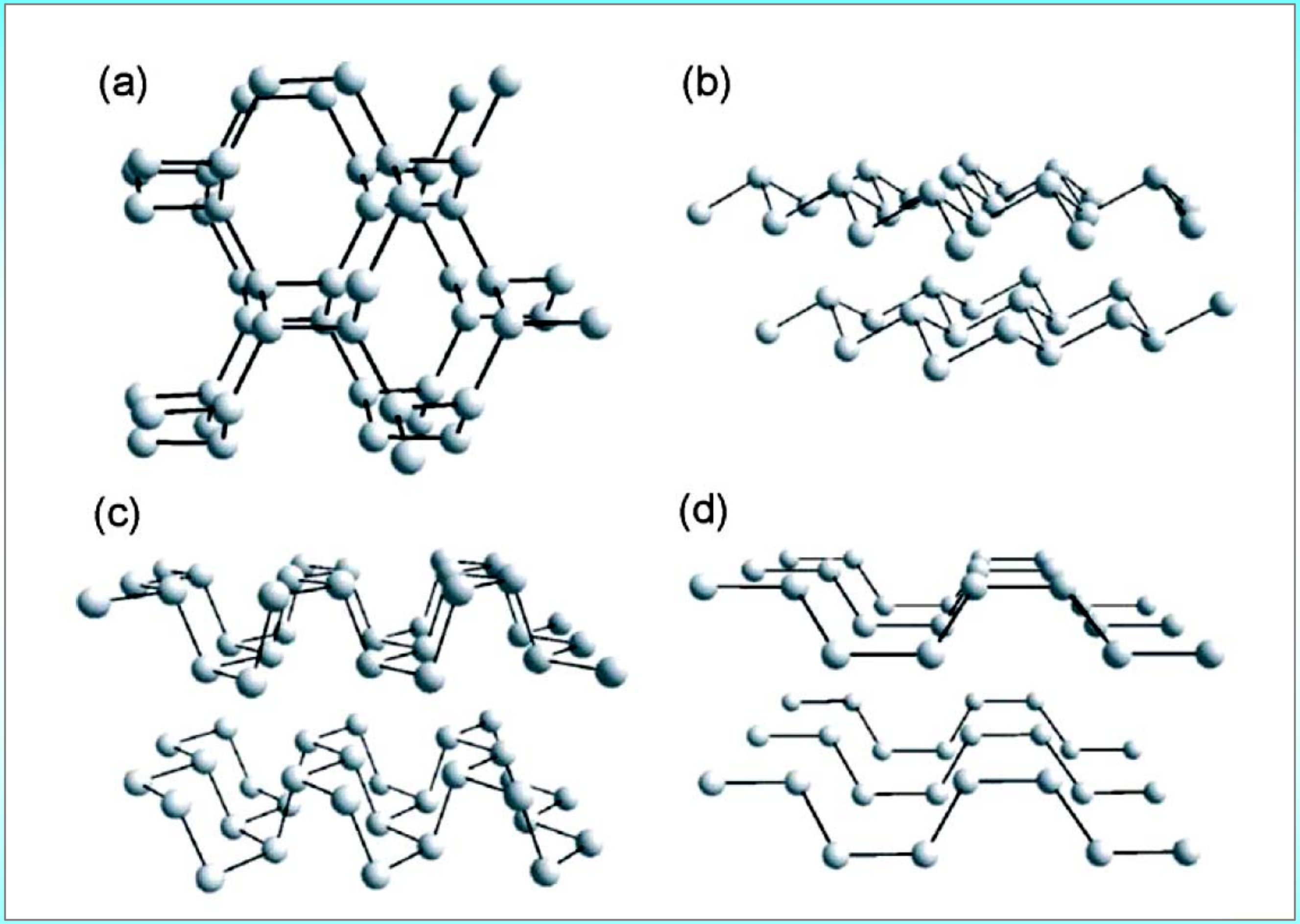
Single covalent bond

D_e= 3.0 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

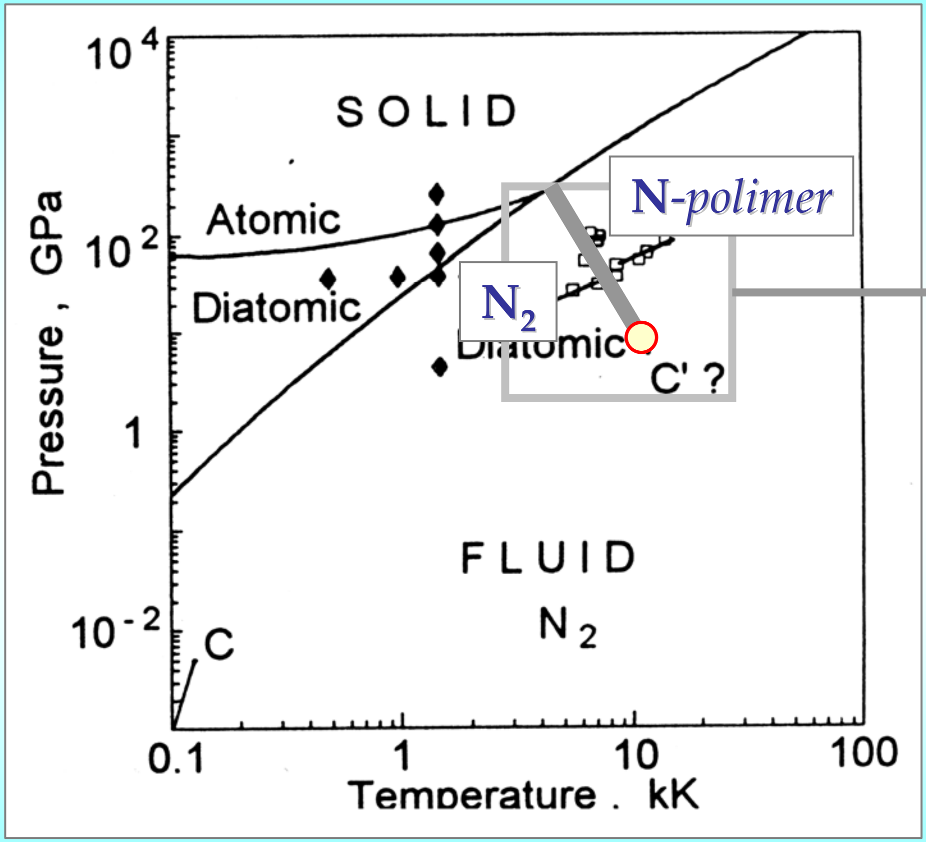
Polymeric nitrogen - structure



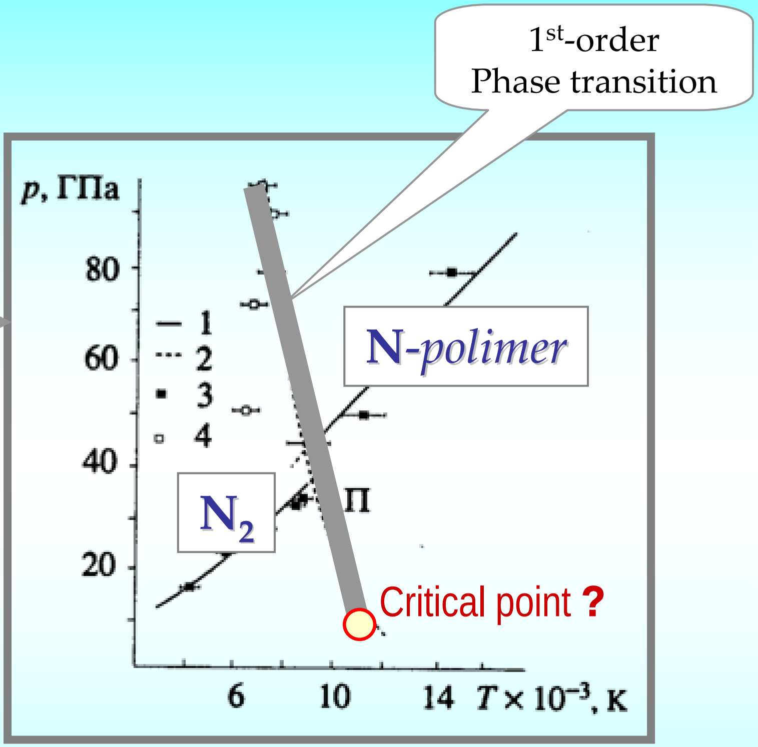
F.Zahariev,A.Hu,J.Hooper,F.Zhang,&T.Woo. Phys.Rev. B 72,214108 (2005)

Simple molecular models

First estimations of molecular-polymeric transition



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



1 - Hugoniot

2 - Phase equilibrium line

Experiment (Nellis ea, 2001)

3 - Single shock

4 - Double shock

Plasma model for nitrogen thermodynamics

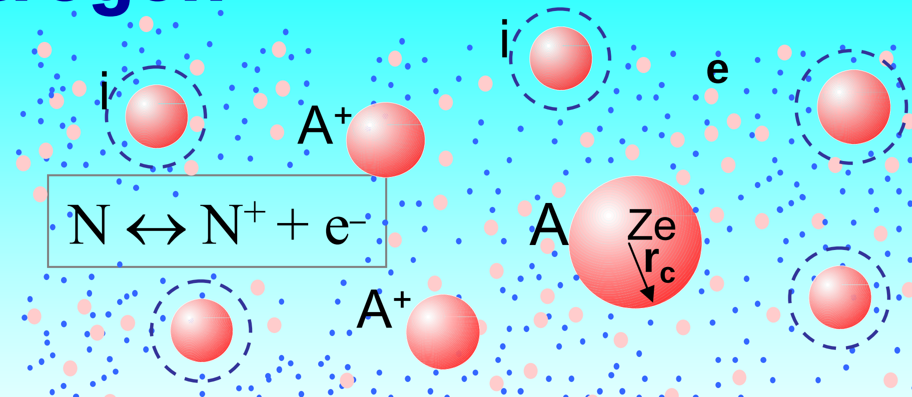
(code SAHA-N)

Shock compression of nitrogen

(chemical picture)

SAHA-code

Gryaznov, Iosilevskiy (1970-2010)



$N_2 \leftrightarrow 2N$ | $N_2^+ \leftrightarrow N + N^+$ | $N^- \leftrightarrow N + e^-$

Equilibrium composition:
$\{N_2, N, N^+, e, N_2^+, N^-\}$

Coulomb interaction:
Modified pseudopotential model for partially ionized plasma
(*I. Iosilevskiy 1980-2010*)

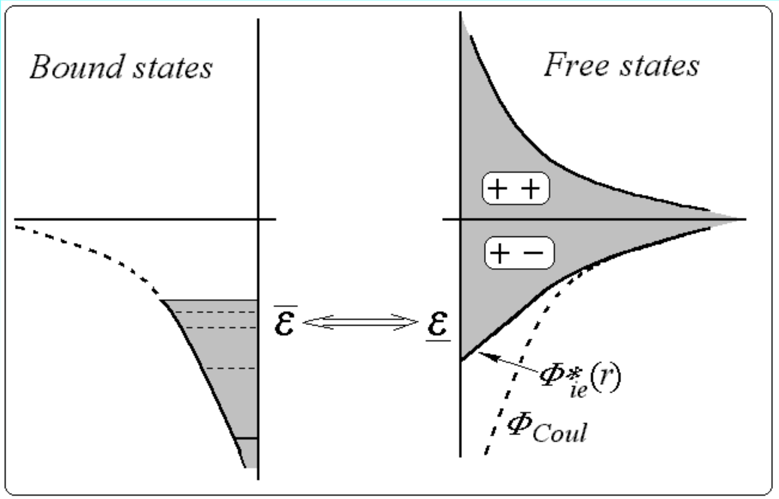
Short range repulsion:
"Soft Spheres" approximation (*D.Young)* modified for *mixture* of soft spheres with *different radii* – shift of dissociation level.

Basic points:
- All assumption are provided at micro-level.
- Input: Choice of Φ_{ie}, Φ_{ii} and Φ_{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.

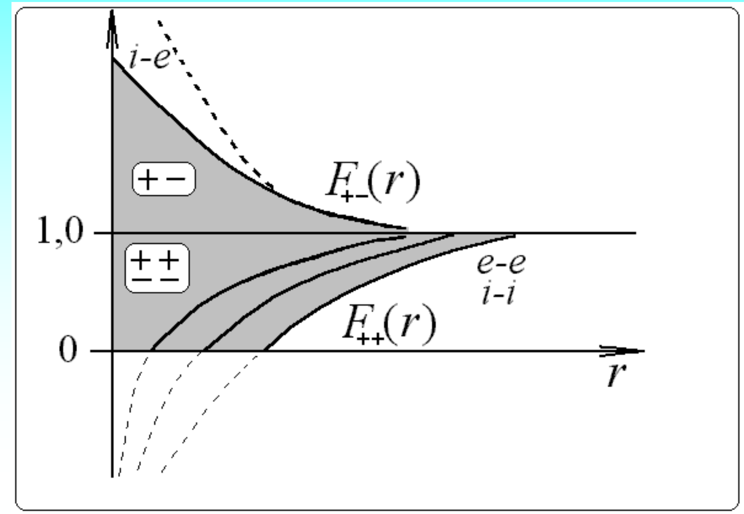
Key parameter – ratio of intrinsic volumes: *molecule /atom / ion:* **$R(N) / R(N_2) = 0.63$**
- in accordance with recommendations of "Atom-atomic approximation" of E.Yakub, *LT, 1993*

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 Glauberman's form (1955))

$$\Phi^*_{\rm ie}(r) = -\frac{Z_{\rm i}e^2}{r}\left(1-{\rm e}^{-r/\sigma}\right) \geq -\varepsilon$$

⇔

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

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

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*)

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

Positive sign of all correlation functions ⇔ $F_{\rm ab}(r) > 0$

(*) 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

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

⇔

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

Pseudopotentials

Correlation Functions

Homogeneity of Coulomb potential ⇔

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

Total Energy correction

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

Potential Energy Correction - ΔU_{Pot}

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

Pressure Correction - ΔP

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

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

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

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 (Γ << 1), is ***no longer valid*** in strong non-ideality conditions (Γ ~ 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 ⇔ Theoretical models

(*comparison*)

Thermodynamics of shock compressed nitrogen

(primary thermodynamic results of experiment)

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

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

Internal energy is almost linear on pressure at isochore

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

Temperature is almost linear on pressure at isochore

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

$$Z \equiv PV/RT \equiv P/n_{\mathrm{N}}kT \approx const \approx 2.66 \pm 0.20$$

Internal energy is almost linear on temperature at isochore

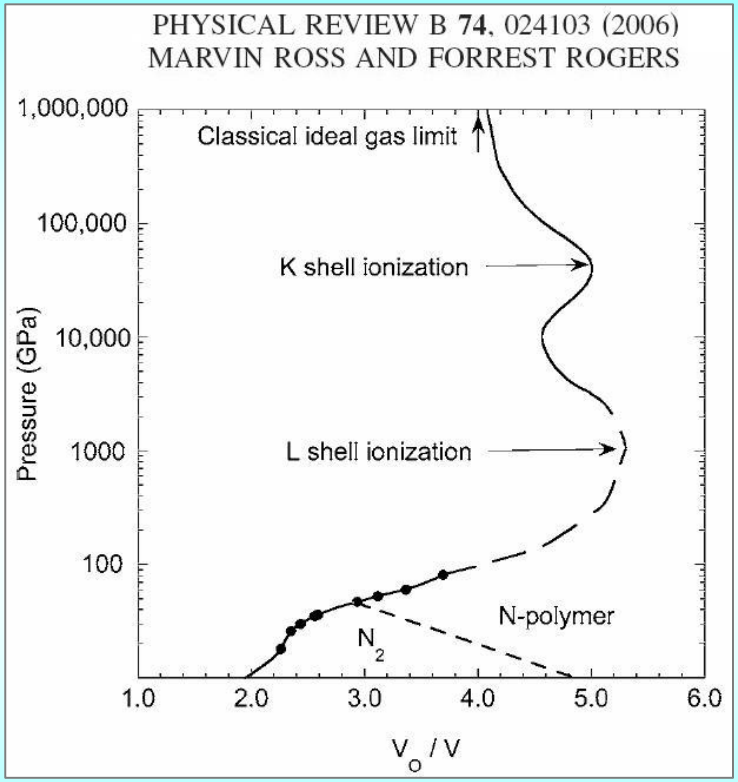
$$C_V \equiv (\partial E/\partial T)_V \approx const \approx 2.06 \text{ (J/g·K)}$$

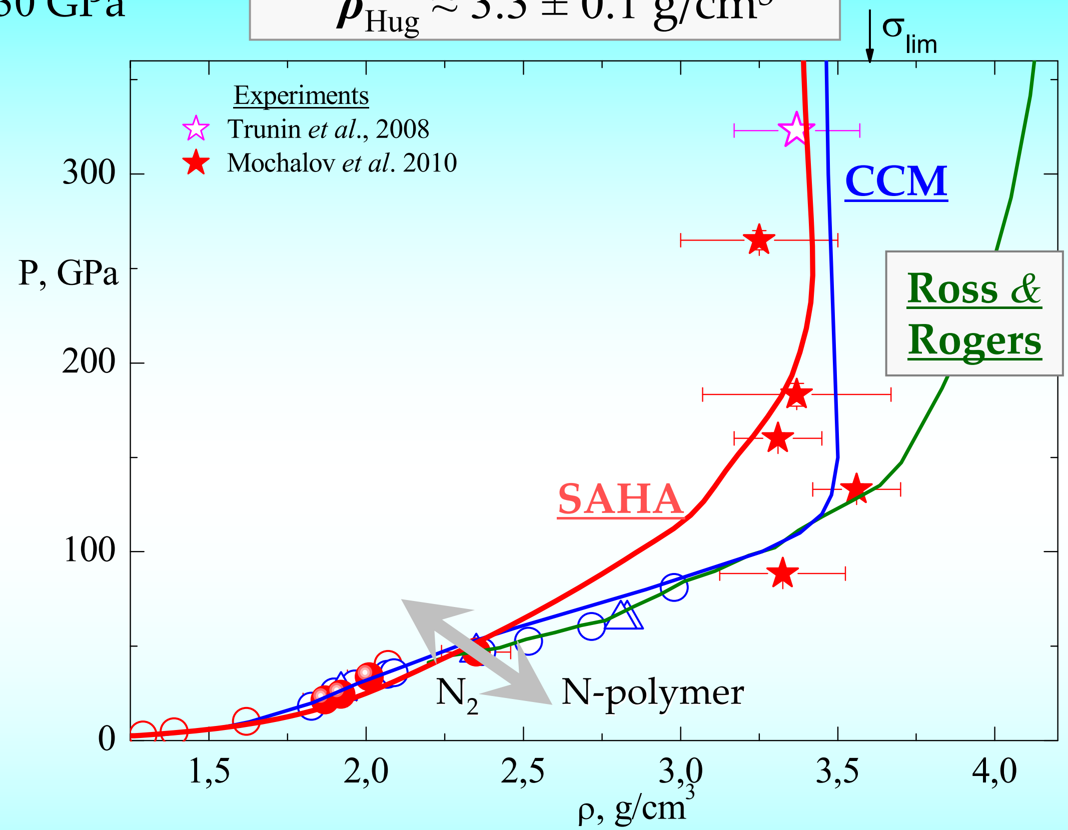
Check of theoretical models

Quasi-isochoric behavior of nitrogen Hugoniot

$90 < P_{Hug} < 330$ GPa

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





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

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

★ - 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**

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

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

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

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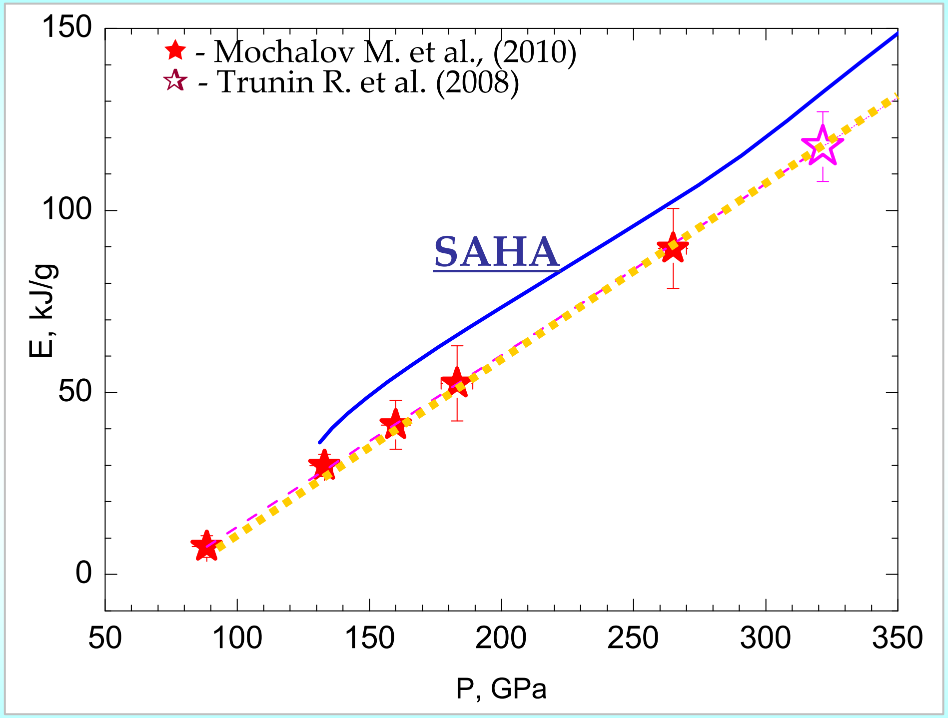
Internal energy is almost linear on temperature at isochore

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

Quasi-linear behavior of $E(p)$ at $\varrho = const$

Hugoniot: $\sim \rho \approx const$ (3.3 ± 0.1 g/cc)

Internal Energy ⇔ 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

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

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

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

Temperature is almost linear on pressure at isochore

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

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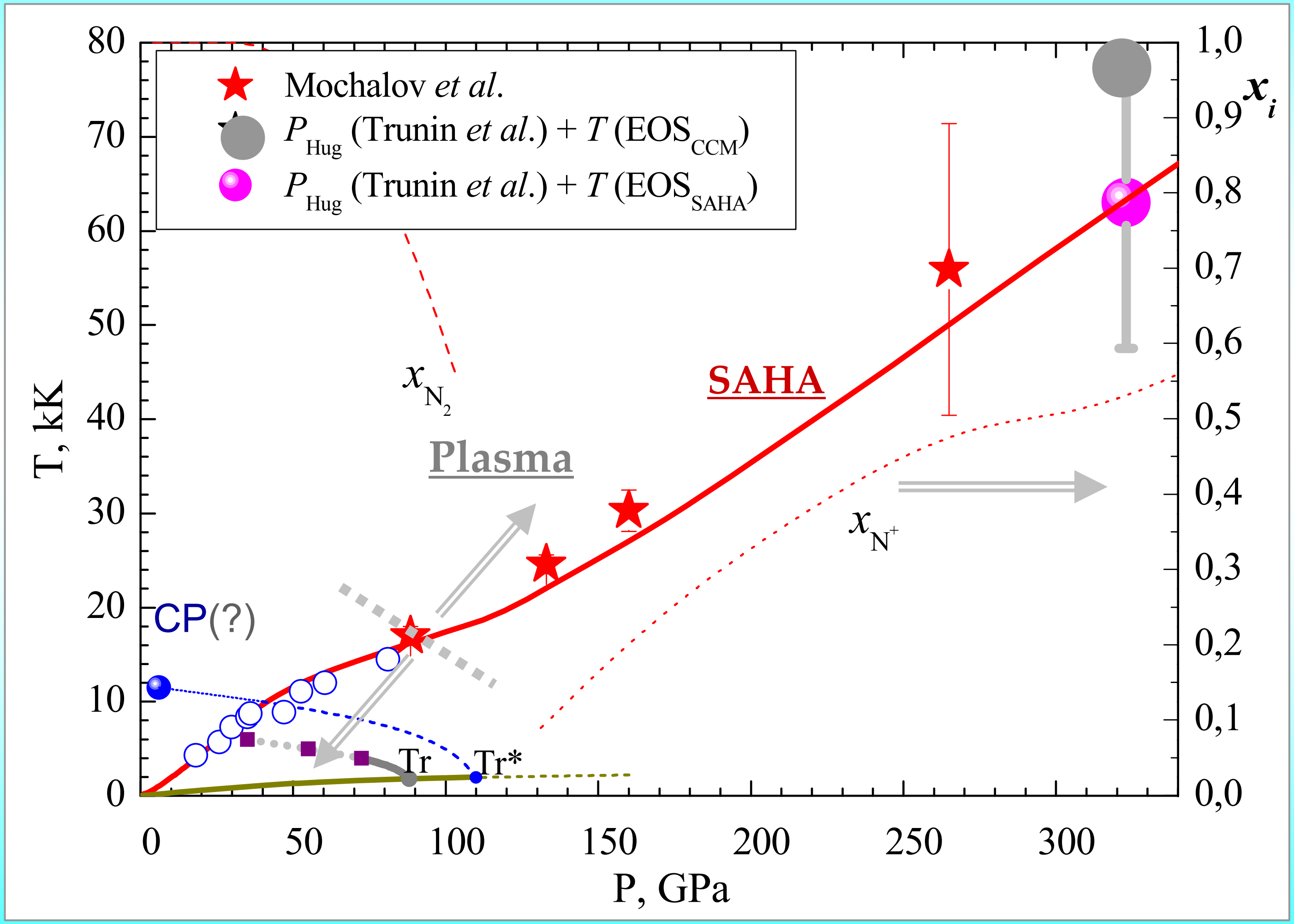
Internal energy is almost linear on temperature at isochore

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

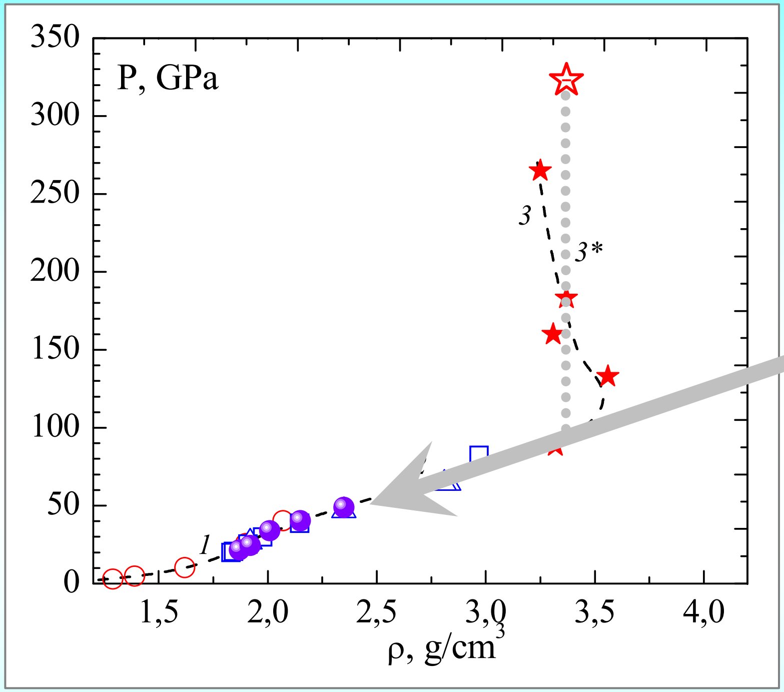
Temperature of shock compressed nitrogen

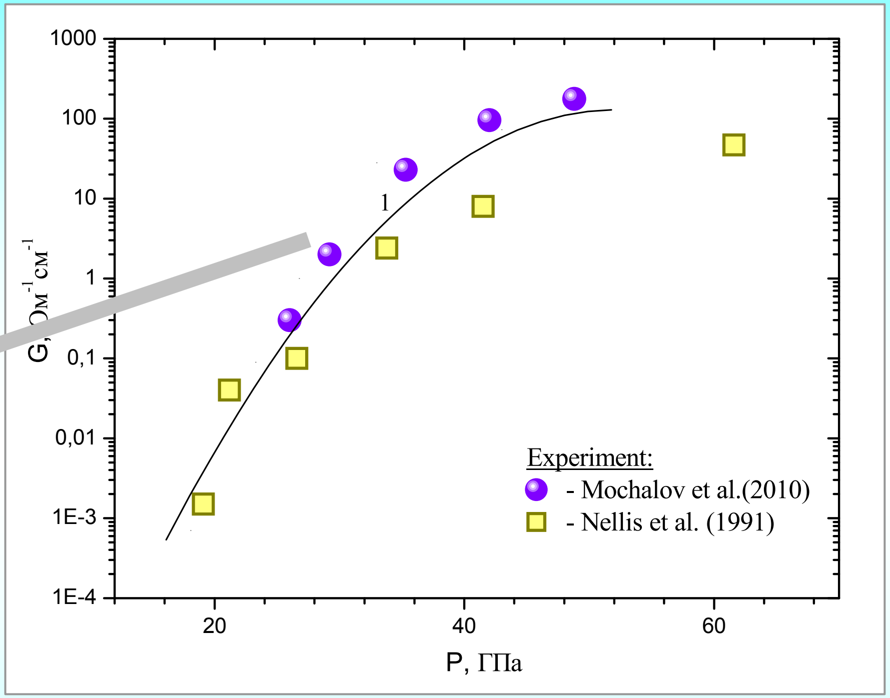
General P-T diagram



Quasi-linear behavior of *T(p)* at ϱ = *const*

Electroconductivity of shock compressed nitrogen

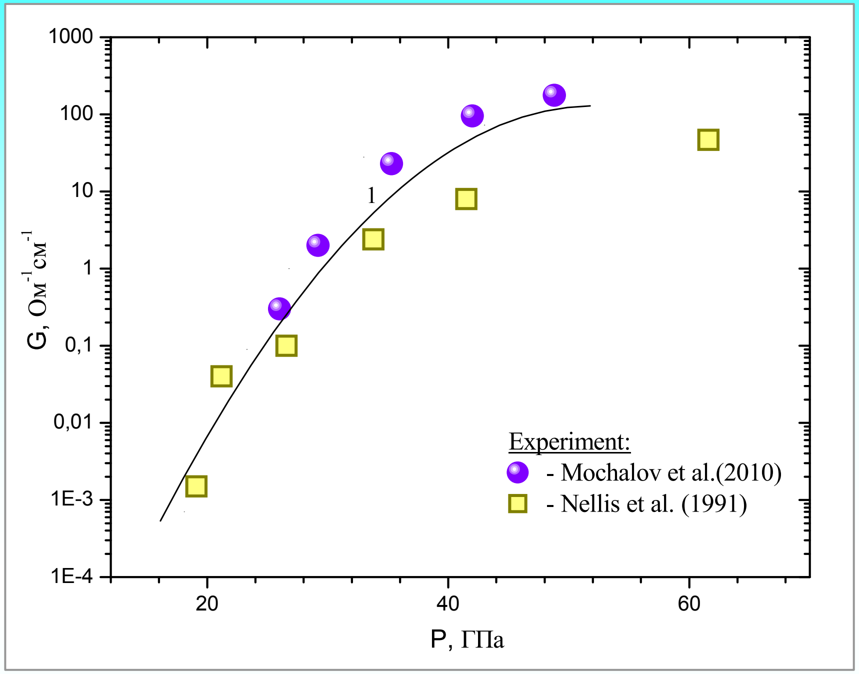


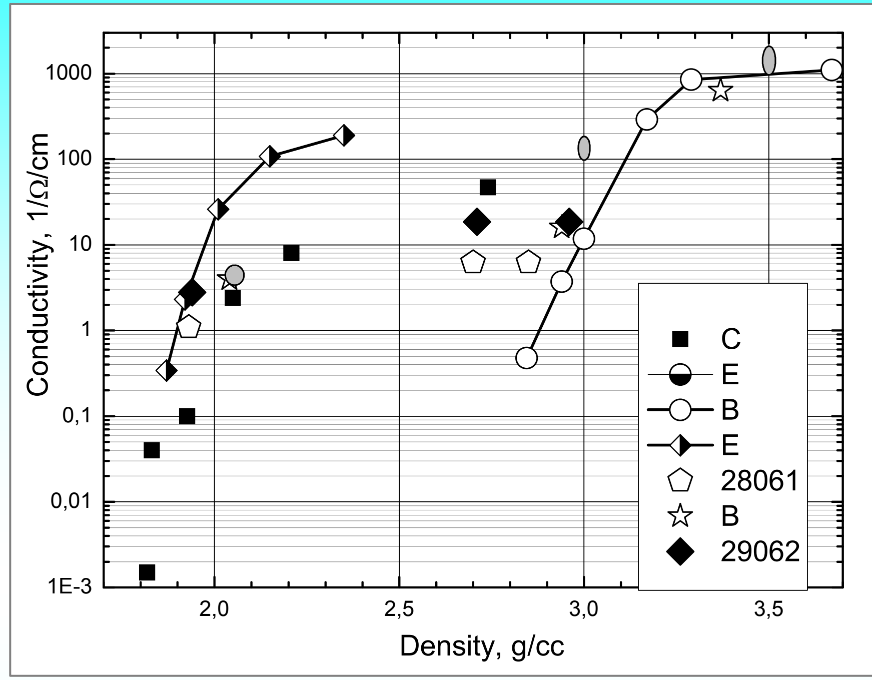


●★ - Experiment /Mochalov M. et al. / *JETF* **137** (2010)

Nellis W., Radovsky H. et al. *J. Chem. Phys*. **94** (1991)

Electroconductivity of shock compressed nitrogen





●★ - Experiment /Mochalov M. et al. / *JETF* **137** (2010)

Ternovoi V. *et al*. (email - 30.05.2010)

Quasi-isentropic Plane Compression of Matter at Megabar Pressures by Using of a Layered System to Diminish First Shock Wave Intensity

Ternovoi V., Pyalling A., Filimonov*et* A. (*05.2010*)

Summary and conclusion

Explosive driven quasi-isentropic compression generators were proposed for matter investigation in the megabar pressure region. Results of the first experiments on quasi-isentropic compression of liquid nitrogen are presented. It was shown, that **pressure ionization** of nitrogen proceeds at **densities** from **3.15 to 3.4 g/cc** at a **temperature** of about **3000 K.** Diminishing of temperature growth was measured during onset of nitrogen electrical conductivity.

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** (*mesurement of series of Hugoniots 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

. . . .

Conclusions

- **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

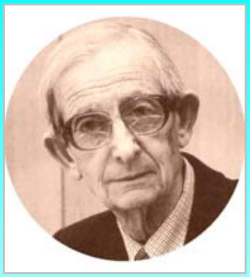
- **Simultaneous** measurement of **caloric** and **thermal** equation of state (EOS) *(pressure, density, temperature and internal energy)* on the same Hugoniot give powerful tool for **checking** theoretical **models** and "calibration" of wide-range EOS*-s*

- **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

- It is **promising** to continue and extend **experimental** investigation of **pressure ionization** of **polymeric** state

- It is **promising** to study **pressure ionization** of **polymeric** state in **direct numerical simulations** ("*numerical experiment*") DFT_MD, PIMC, WP_MD…



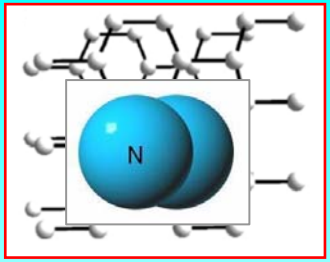
Sarov, 2011

Annual Moscow Workshop

Non-ideal Plasma Physics

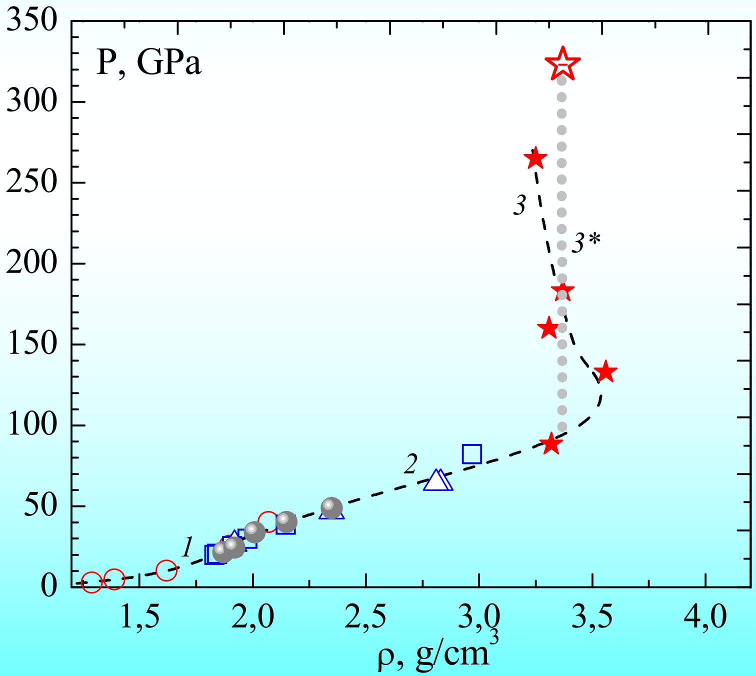
Russian Academy of Science

November 23-24, 2011



Chernogolovka, 2010
EMMI, GSI, 2011

Thank you!



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and by **MIPT Education Center** “Physics of High Energy Density Matter” and by **Extreme Matter Institute (EMMI)**