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Droplet evolution in a liquid/vapor aluminum flow

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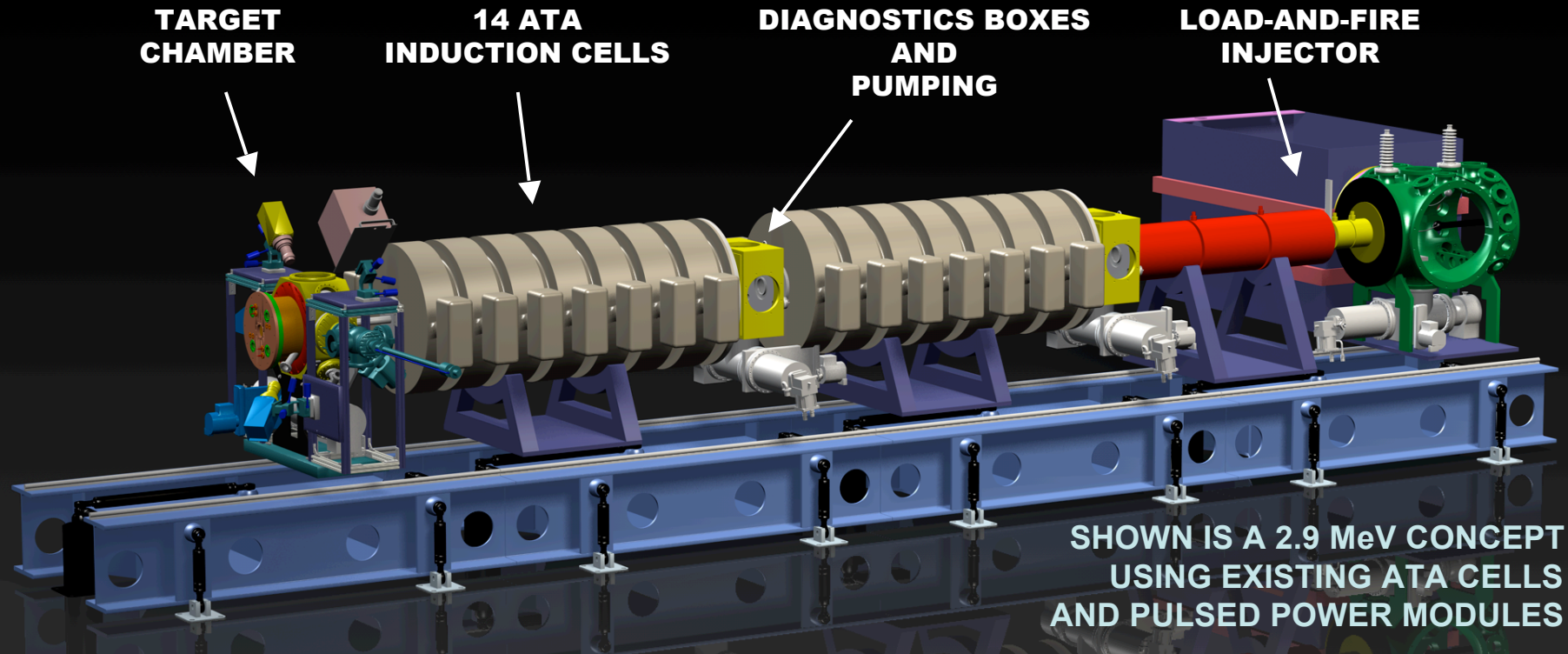
Abstract

We have made estimates of surface effects and droplet evolution in the two-phase flow that should be observed in the upcoming foil heating experiments planned for the NDCXII machine at LBNL. An aluminum foil of order micron thickness will be heated by a heavy ion beam to the 1 eV range. The expansion will take place in the two-phase regime (gas/liquid), so the heated metal will first melt, then fragment into droplets, and then the droplets will undergo some evaporation. We propose hydrodynamic criteria to estimate the maximum size of the droplets (~ 100 nm), considering a balance between hydrodynamic disruptive forces and restoring surface tension. We estimate the relevant thermodynamic functions (surface tension, latent heat, viscosity) for temperatures up to the critical temperature, and we use them to make a simple model for the partial or total evaporation of a droplet in the expanding flow.

Outline

1. Introduction: Warm Dense Matter (WDM) studies
2. Expected qualitative hydrodynamics of metals expanding in a two-phase flow. Maximum size of droplets.
3. Estimates of needed physical quantities:
 - σ - surface tension
 - L - latent heat
 - μ - viscosity
4. Dynamic evolution of droplets. Governing equations.
 1. Low temperature case ($< \sim T_c = \text{critical temperature}$)
 2. High temperature case ($> T_c$)

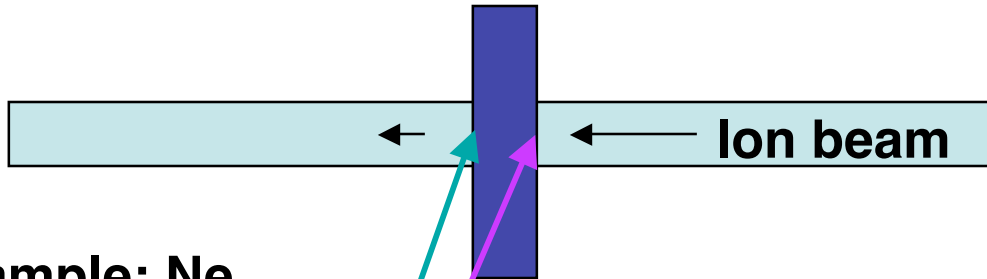
NDCX II is a planned accelerator designed to reach uniform warm dense matter conditions



Ion Beam	A	Energy at Bragg Peak	dE/dX at Bragg Peak	Foil Entrance Energy (approx)	Δz for 5% variation (10% solid Al)	Beam Energy for T=10 eV/mm ²	t_{hydro} at 10 eV	Beam Power per mm ²	Beam Current for 1 mm diameter spot	Line Charge Density at Focus	Density at Focus
	amu	MeV	MeV-cm ² /mg	MeV	μm	J/mm ²	ns	GW/mm ²	A	C/m	cm ⁻³
Li	6.94	1.9	2.05	2.9	34.3	5.7	0.8	6.8	1860.7	2.09E-04	1.66E+15
Na	22.99	15.9	11	23.9	53.5	8.9	1.3	6.8	222.3	1.57E-05	1.25E+14
K	39.10	45.6	18.6	68.4	90.8	15.1	2.2	6.8	77.5	4.22E-06	3.35E+13

Strategy: maximize uniformity and the efficient use of beam energy by placing center of foil at Bragg peak

In simplest example, target is a foil of solid or “foam” metal



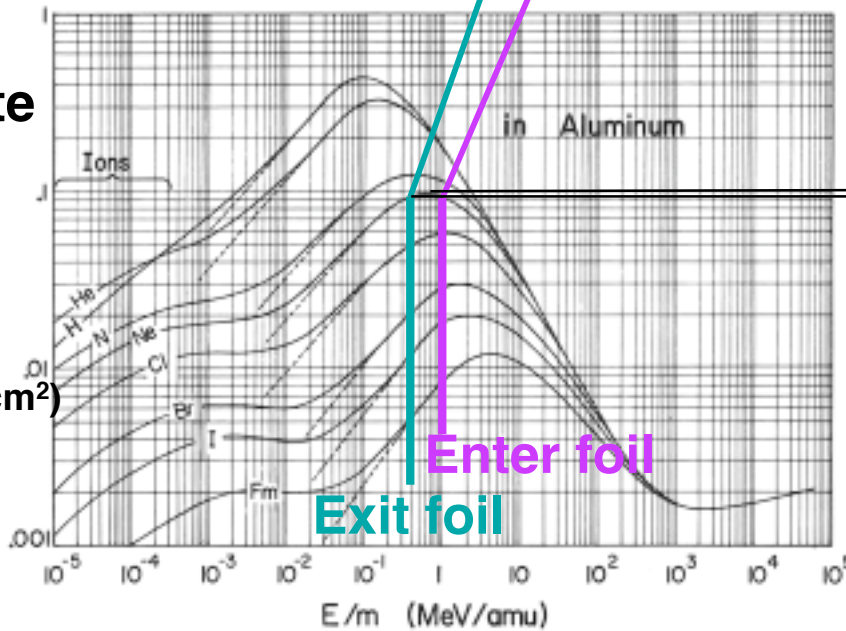
fractional energy loss can be high and uniformity also high if operate at Bragg peak (cf. [1])

Example: Ne

Energy loss rate

$$-\frac{1}{Z^2} \frac{dE}{dX}$$

(MeV/mg cm²)



$$\Delta dE/dX \propto \Delta T$$

In example,

$$E_{\text{entrance}} = 1.0 \text{ MeV/amu}$$

$$E_{\text{peak}} = 0.6 \text{ MeV/amu}$$

$$E_{\text{exit}} = 0.4 \text{ MeV/amu}$$

$$(\Delta dE/dX)/(dE/dX) \approx 0.05$$

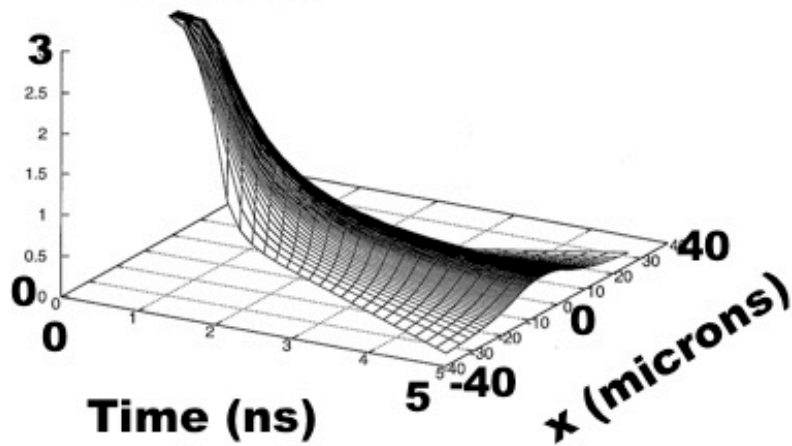
Energy/ion mass (MeV/amu)

(dEdX figure from [2])

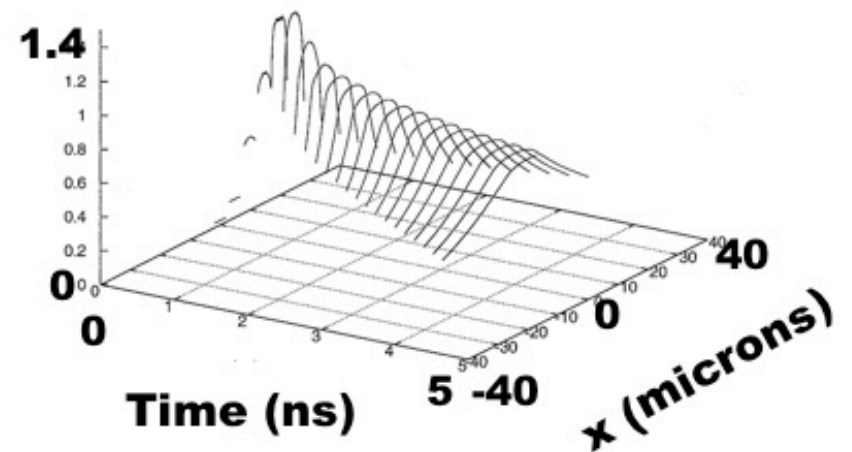
Two-phase WDM target hydrodynamics

ρ and T evolution of a plane WDM target (DPC simulation result) (cf. [3])

Density (g/cc)



Temperature (eV)

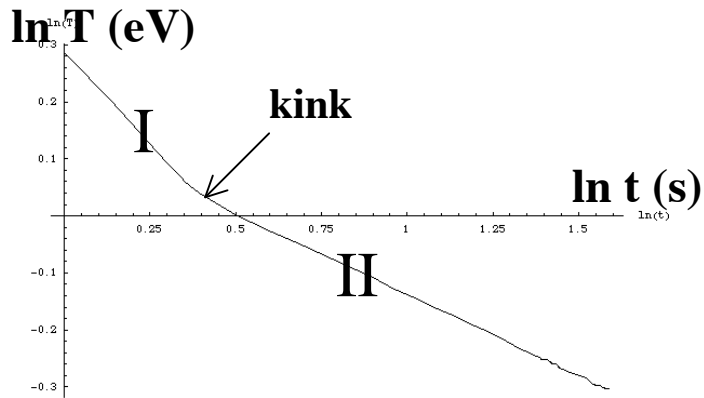


Reference case:

beam: Li⁺ at 2.8 Mev/ion
target: 3.5 μm -thick aluminum foil
pulse length: 1 ns
focal spot: \sim 1 mm

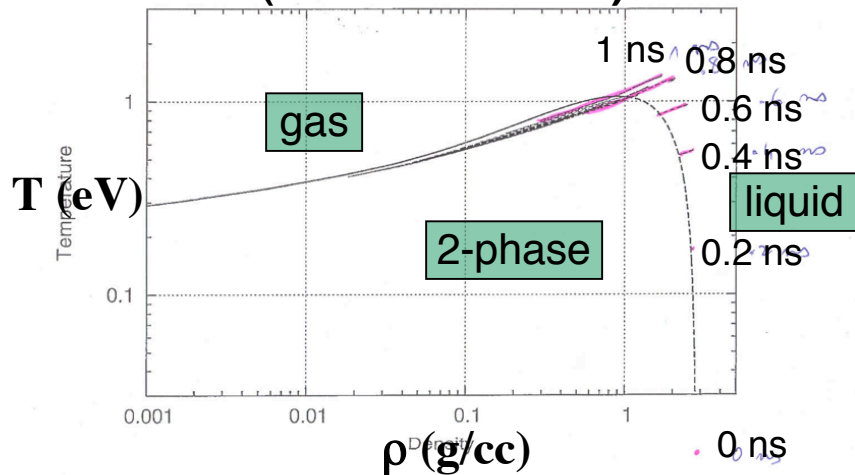
Discontinuity in temperature decay power law has motivated investigation of 2-phase behavior

(* Temperature decay from 1 to 5 ns for Ref case *)

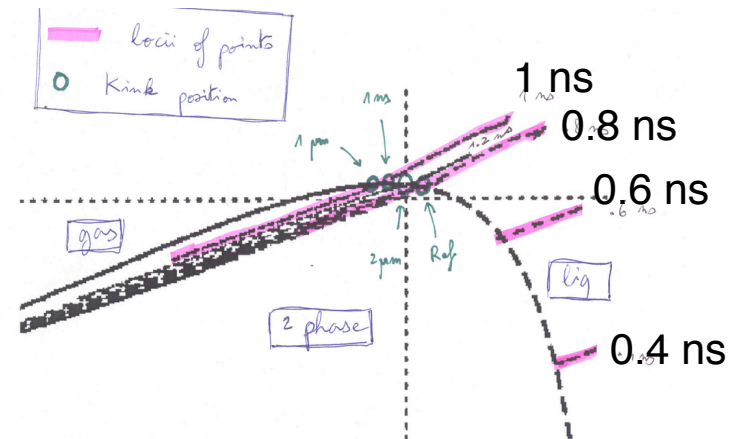


- Fast decay (I: approx $-2/3$) and then slow decay (II: approx $-1/3$)
- Change in slope (kink) corresponds to moment when center of the foil enters the 2-phase region

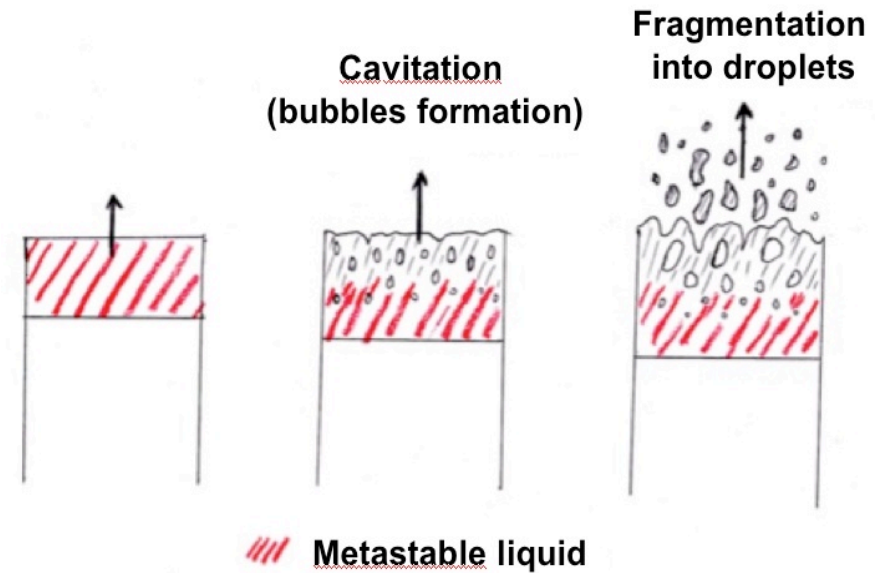
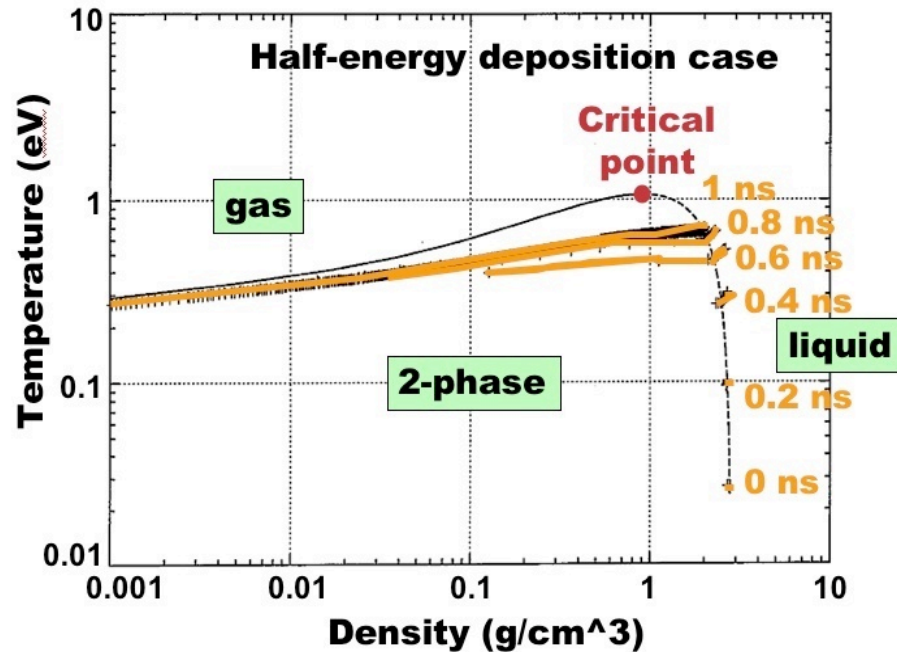
From liquid to 2-phase regime
(reference case)



Position of kink: on the border

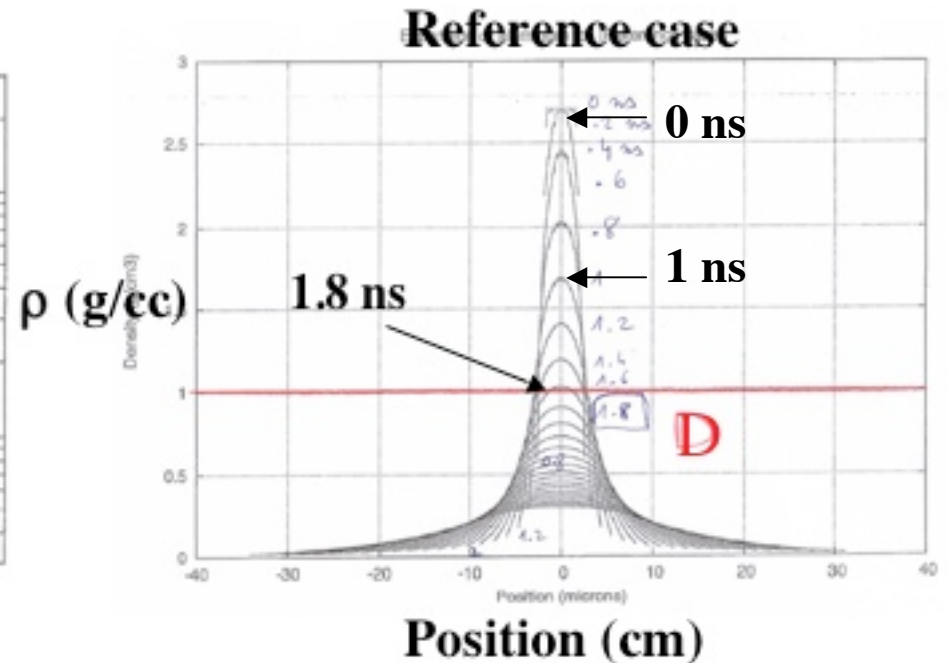
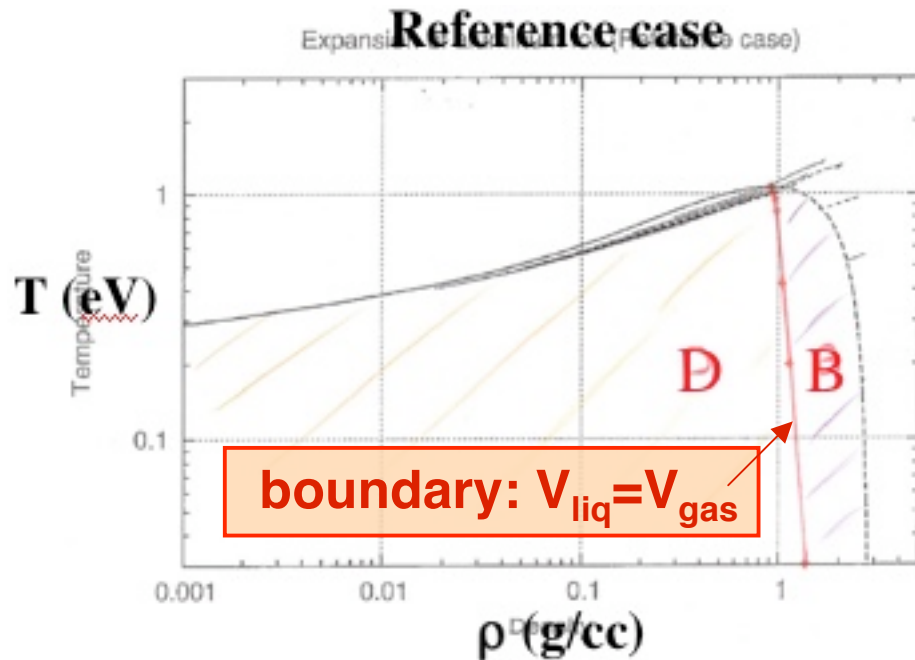


How can we describe the 2-phase hydrodynamics?



- The foil will melt then enter 2-phase conditions.
- First, bubble form (B), then the continuous liquid fragments into droplets (D)

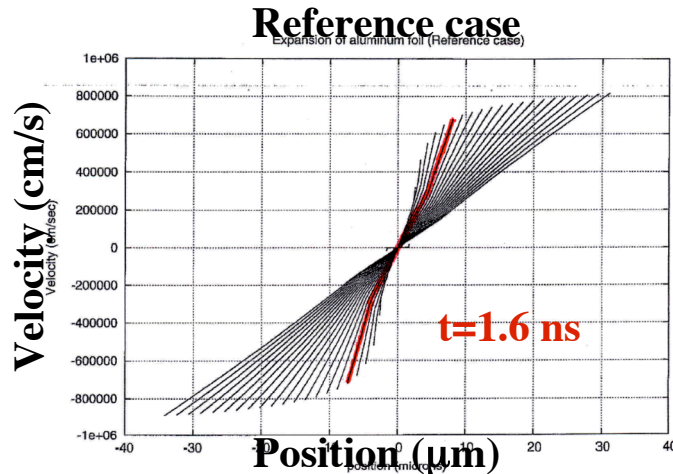
Bubbles or droplets?



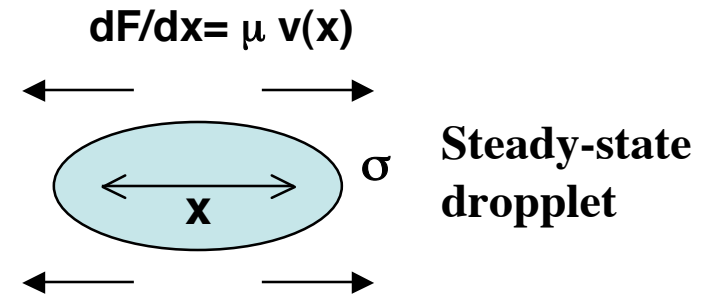
Separation line is where each phase occupies half of the volume

First bubbles form, but then quickly droplets form everywhere,
(always for $\rho < \sim 1 \text{ g/cm}^3$, for these parameters)

Maximum size of a droplet in a diverging flow ?



Locally, $dv/dx = \text{const}$
(Hubble flow)



❖ Equilibrium between stretching viscous force and restoring surface tension:
Capillary number $Ca = \text{viscous/surface} \sim \int \mu dv/dx \cdot x \cdot dx / (\sigma x) \sim (\mu dv/dx x^2) / (\sigma x) \sim 1$

→ Maximum size : $x = \sigma / (\mu dv/dx)$ (cf. [4], [5])
→ Estimate : $x_{\text{max}} \sim 0.2 \mu\text{m}$

AND/OR:

❖ Equilibrium between disruptive dynamic pressure and restoring surface tension: **Weber number** $We = \text{inertial/surface} \sim (\rho v^2 A) / \sigma x \sim \rho (dv/dx)^2 x^4 / \sigma x \sim 1$

→ Maximum size : $x = (\sigma / \rho (dv/dx)^2)^{1/3}$ (cf. [6])
→ Estimate : $x_{\text{max}} \sim 0.05 \mu\text{m}$

Typical parameters for max size calculation

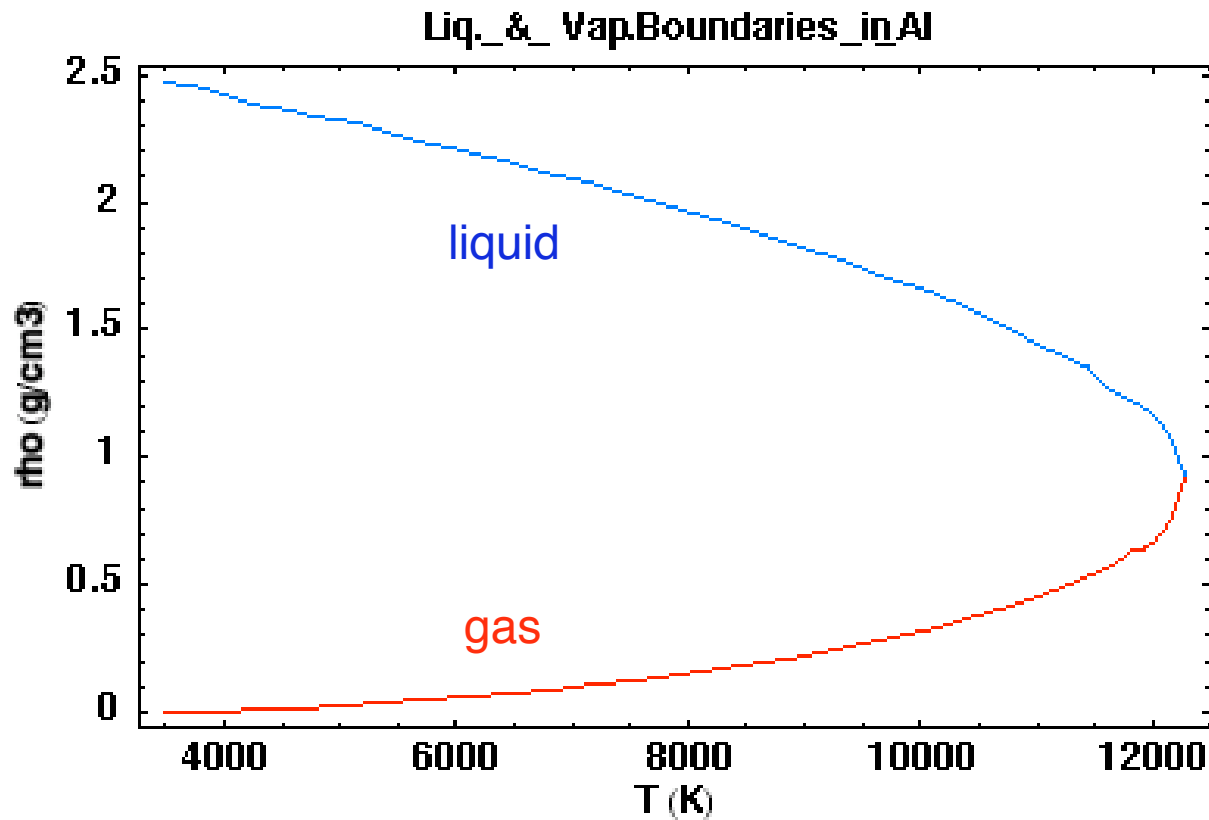
Typical conditions for droplet formation:

$t=1.6 \text{ ns}$, $T=1 \text{ eV}$, $\rho_{\text{liq}}=1 \text{ g/cm}^3$

- **Surface tension:** $\sigma \approx 100 \text{ dyn/cm}$
- **Thermal speed:** $v \approx 5 \cdot 10^5 \text{ cm/s}$
- **Viscosity:** Kinetic gas: $\mu = \frac{1}{3} m v \cdot n l$
mean free path : $l = \frac{1}{\sqrt{2} n \sigma_0}$
 $\rightarrow \mu = m v / (3 \sqrt{2} \sigma_0) = 27 \cdot 1.67 \cdot 10^{-24} \cdot 5 \cdot 10^5 / (3\sqrt{2} \cdot 10^{-16})$
 $\mu \approx 5 \cdot 10^{-3} \text{ g/(cm-s)}$
- **Velocity gradient:** $dv/dx = 10^6 \text{ cm/s} / 10^{-3} \text{ cm}$
 $dv/dx = 10^9 \text{ s}^{-1}$

→ Conclusion: Maximum size is expected to be $\sim 0.1 \mu\text{m}$

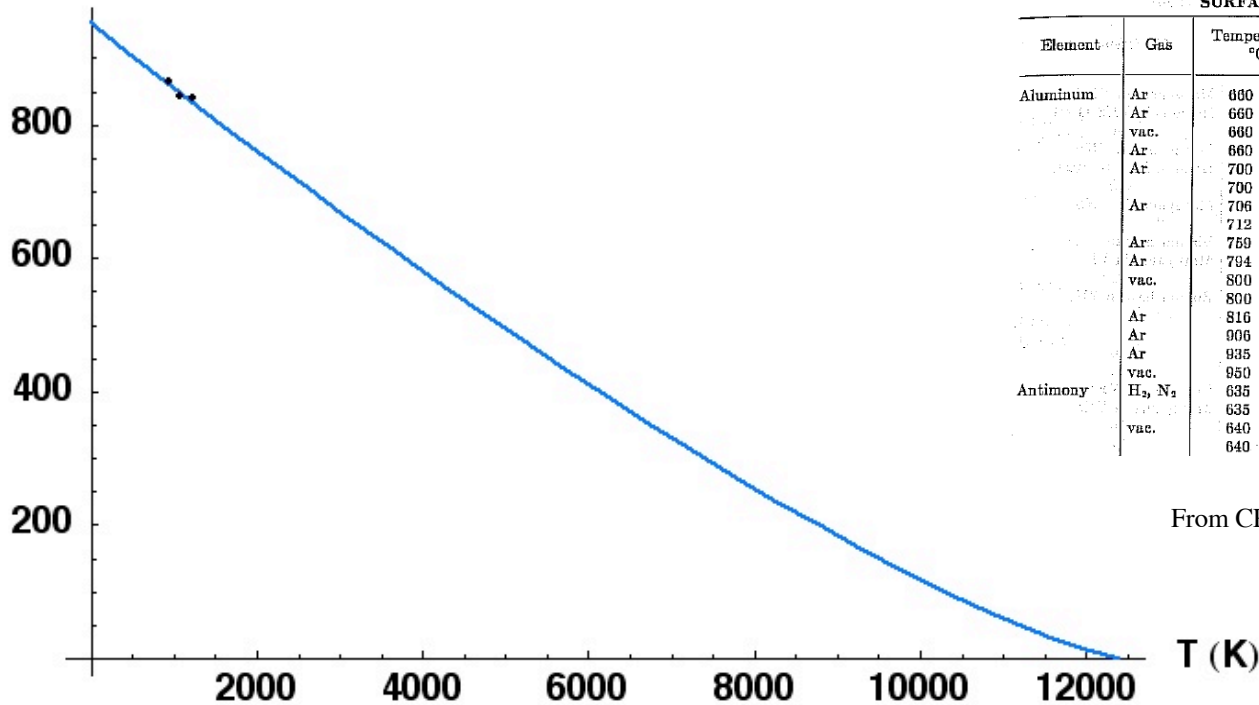
Liquid and vapor density boundary in Al



Taken from the EOS used in the DPC code : obtained by maxwellian construction

Surface tension of liquid aluminum

sigma (dyn/cm) Surface tension of liquid Aluminum



SURFACE TENSION OF LIQUID ELEMENTS					
Element	Gas	Temperature °C	Dynes/cm	Method	References
Aluminum	Ar	660 (m.p.)	860	Bubble pressure	5
	Ar	660	914	"	Zhivov in VKS (1937)
	vac.	660	865	Sessile drop	8
	Ar	660	825	Bubble pressure	59
	Ar	700	850	"	4
		700	900		
	Ar	706	494	Bubble pressure	Pelzel in VKS (1947)
		712	502		Zhivov in VKS (1937)
	Ar	759	489	Bubble pressure	Klyachko in VKS (1937)
	Ar	794	483	"	Zhivov in VKS (1937)
	vac.	800	845	Sessile drop	6
		800	865		Pelzel in VKS (1947)
	Ar	816	480	Bubble pressure	Zhivov in VKS (1937)
	Ar	906	460	"	"
Ar	935	463	"	"	
Antimony	vac.	950	840	"	7
	H ₂ , N ₂	635	383	"	16
		635	383		Greenaway in VKS
	vac.	640	367.9	Drop weight	15
		640	349		Bircumshaw in VKS

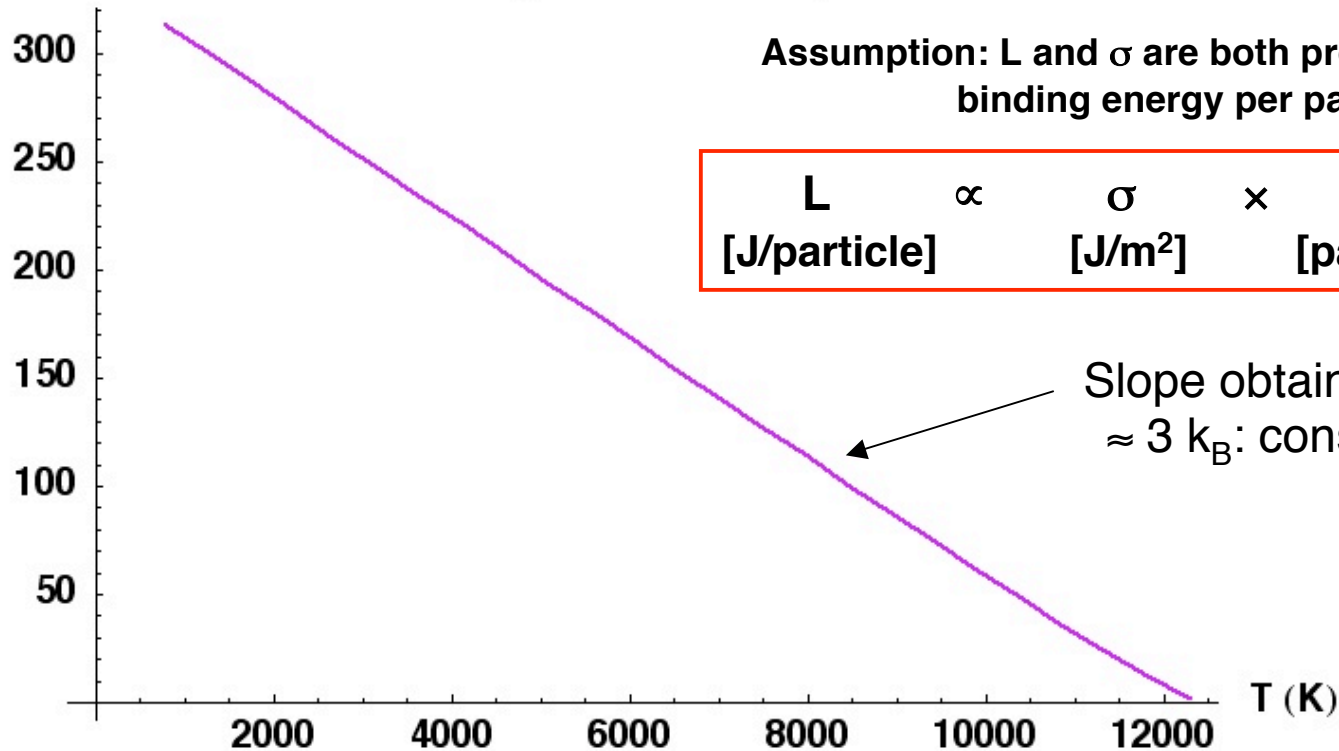
From CRC Handbook in chemistry and physics (1964)

Curve obtained by fitting universal law for simple liquids (**principle of corresponding states**) with data at low temperature and value of critical temperature T_c (cf. [7])

$$\sigma = \sigma_0 (1 - T/T_c)^{1+r} \quad \text{with } r = 0.27$$

Latent heat is nearly linear

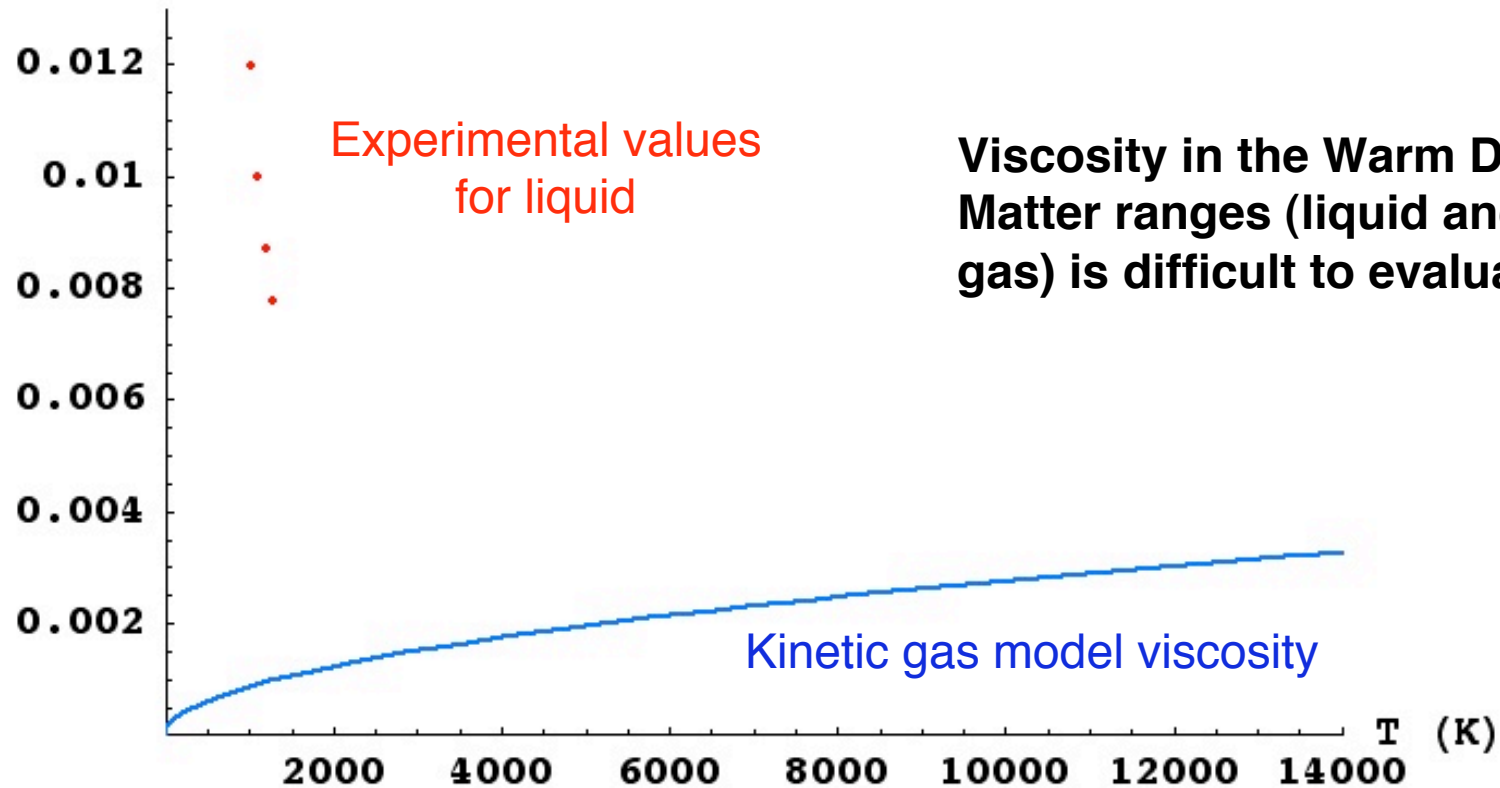
L (kJ/mol) Latent heat of vaporization of liquid Aluminum



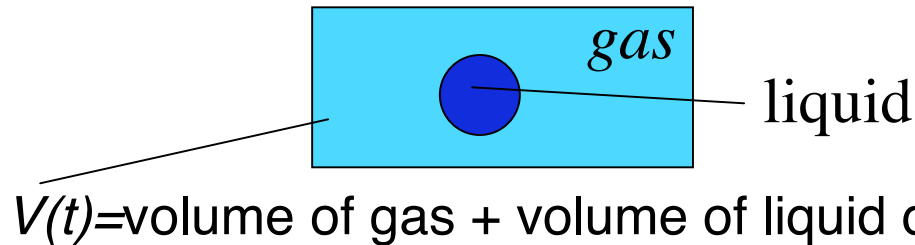
Curve obtained by multiplying $\sigma(T)$ (see previous slide) by $\rho^{-2/3}$ (taken from EOS in DPC) and adjusting with experimental value at low temperature

Viscosity of liquid and vaporized Aluminum

viscosity (g/cm.s)



Model equations for evaporation and condensation of droplets (preliminary equations)



$\rho_g(T)=mn_g(T)$ and $\rho_l(T_l)=mn_l(T_l)$ taken from 2-phase boundary in EOS

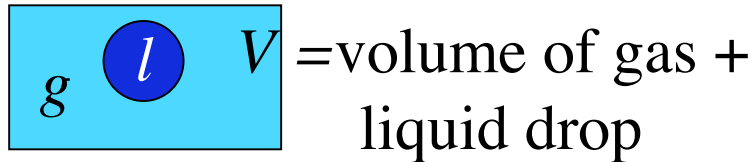
Kelvin's equation: $\ln(P_{curved}/P_{flat})=2\sigma/(n_l k T R_l)$
 $\rightarrow n_{gsat}=n_g(T_l)\exp[2\sigma/(n_l k T_l R_l)]$

Contains all the physics of surface effects for the droplets!

kinetic theory of gases

$\Phi_{cond}(m_g, T_g) = m_g/(mV_g) (k_B T_g/2\pi m)^{1/2}$ = flux of particles onto droplet
 $\Phi_{vap}(T_l) = n_{gsat}(T_l) (k_B T_l/2\pi m)^{1/2}$ = flux of particles evaporating off of droplet
 $V_l(m_l, T_l) = 4\pi R_l^3/3 = m_l/(mn_l(T_l))$
 $S_l = 4\pi R_l^2; \quad V_g(m_l, T_l, t) = V(t) - V_l(m_l, T_l)$

Model equations



m_l, T_l = mass, temperature of liquid drop;

m_g, T_g = mass, temperature of gas;

m = atomic mass of material;

α = thermalization coefficient;

β = sticking coefficient;

c_{vg} = heat capacity of the gas = $3/2 k_B$

c_{vl} = heat capacity of the liquid = $3 k_B$

$$1) \frac{d}{dt} (m_l + m_g) = 0$$

mass conservation

$$2) \frac{dm_l}{dt} = m\beta(-\phi_{\text{vap}} + \phi_{\text{cond}})S_l$$

vaporization condensation

$$3) \frac{d}{dt} \left(\frac{m_l}{m} c_{vl} T_l \right) = \left[\beta \left(\underbrace{-(L_0 + c_{vg} T_l)}_{\text{vaporization}} \phi_{\text{vap}} + \underbrace{(L_0 + c_{vg} T_g)}_{\text{condensation}} \phi_{\text{cond}} \right) + \underbrace{(1 - \beta)\alpha}_{\text{thermalization by non-sticking particles}} \phi_{\text{cond}} c_{vg} (T_g - T_l) \right] S_l$$

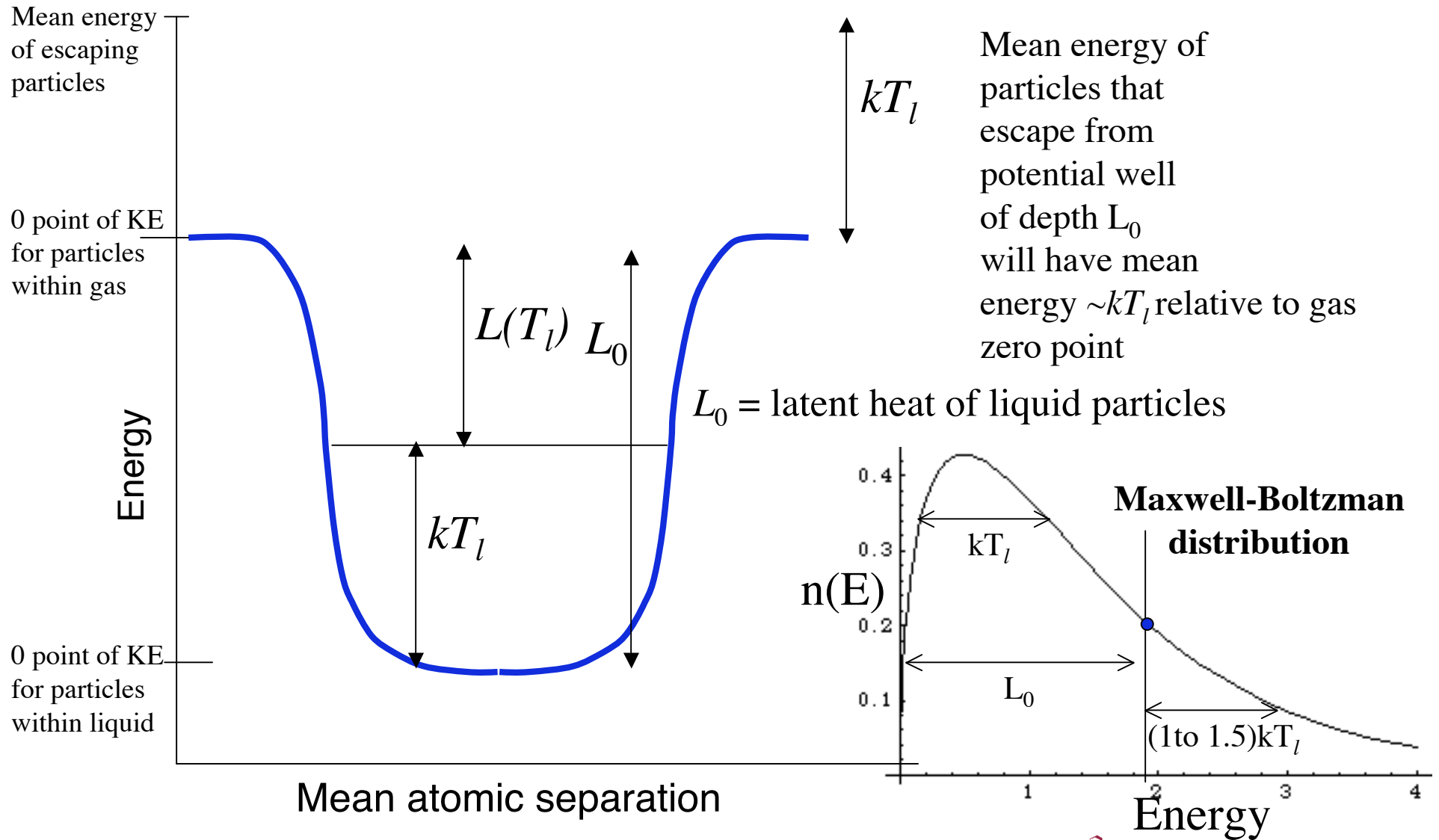
$$4) \frac{d}{dt} \left(\frac{m_g}{m} c_{vg} T_g \right) = \left[\beta \left(\underbrace{c_{vg} T_l}_{\text{vaporization}} \phi_{\text{vap}} - \underbrace{c_{vg} T_g}_{\text{condensation}} \phi_{\text{cond}} \right) - \underbrace{(1 - \beta)\alpha}_{\text{thermalization by non-sticking particles}} \phi_{\text{cond}} c_{vg} (T_g - T_l) \right] S_l +$$

$$+ \frac{\partial E}{\partial V_g} \frac{\partial V_g}{\partial t} + \frac{\partial E}{\partial V_g} \frac{\partial V_g}{\partial m_g} \frac{\partial m_g}{\partial t} \rightarrow + \frac{(1 - \gamma) m_{g0} c_{vg} T_{g0}}{m} V_g(t)^{-\gamma} \left(\frac{dV_g}{dt} - \frac{V_g(t)}{m_g} \frac{dm_g}{dt} \right)$$

prescribed adiabatic expansion

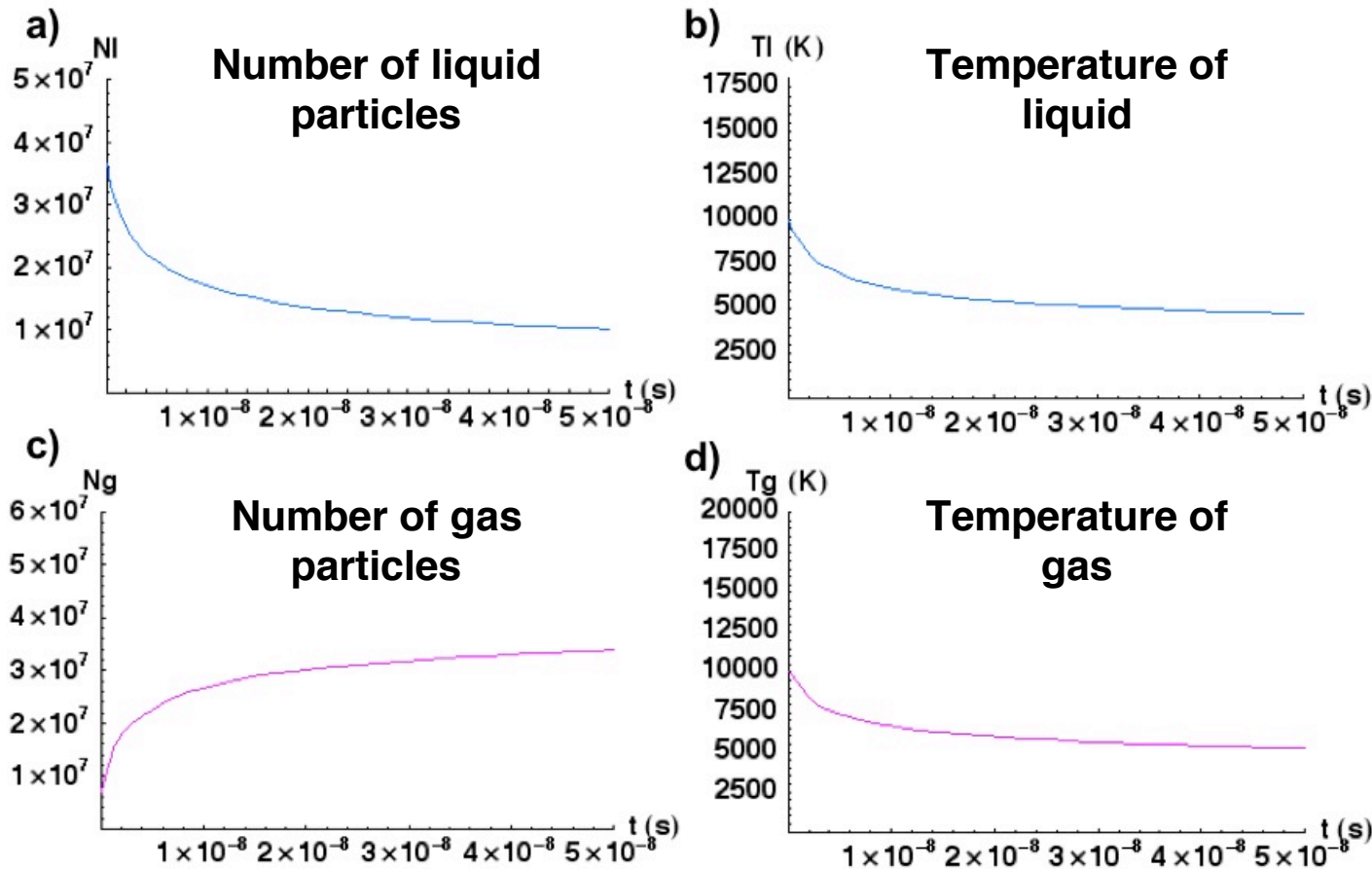
compression heating by vaporizing gas

Why do escaping particles take away $L_0 + c_{vg}T_l$ from liquid?



1. Low initial temperature ($T < T_c$): results of the Mathematica model for the evaporation of a droplet

Assumptions: $\alpha=0.5, \beta=0.5$; at $t=0$: $V_{g0}=V_{l0}=4\pi X_0^3/3$; $X_0=0.1 \mu\text{m}$; $T_{g0}=T_{l0}=10000\text{K}$

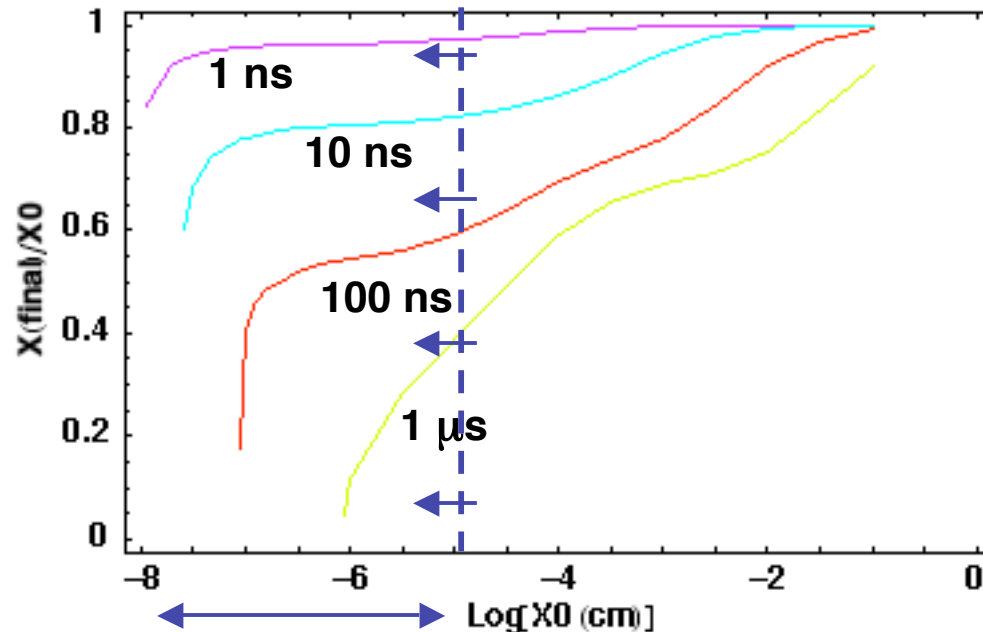


It says... droplets do not evaporate completely \rightarrow

Persisting "bullets" (?)

Model equations show that very small droplets evaporate, whereas larger ones persist

Ratio of final to initial droplet radius vs. initial radius (for 4 different integration times)



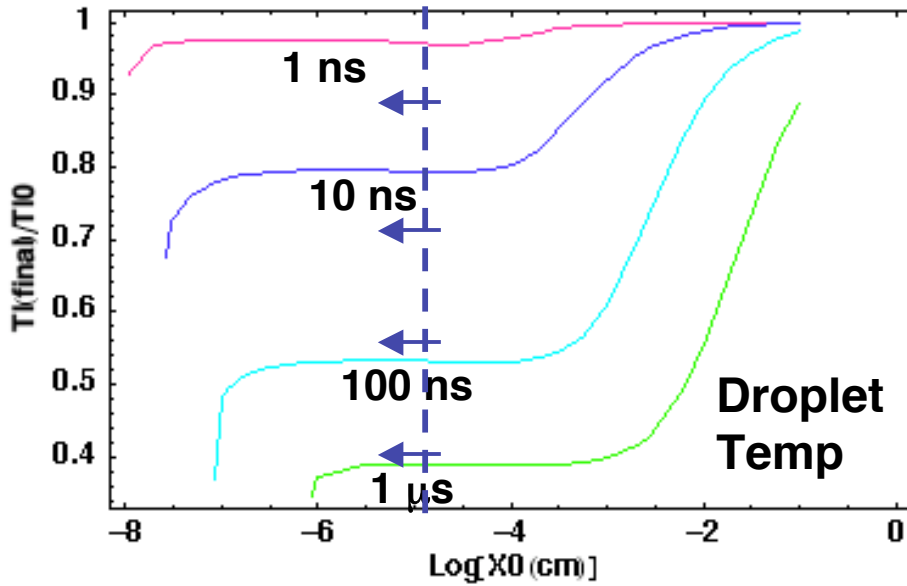
Distance travelled
($v = 500\,000 \text{ cm/s}$):

1 ns	→ 5 μm
10 ns	→ 50 μm
100 ns	→ 500 μm
1 μs	→ 5 mm

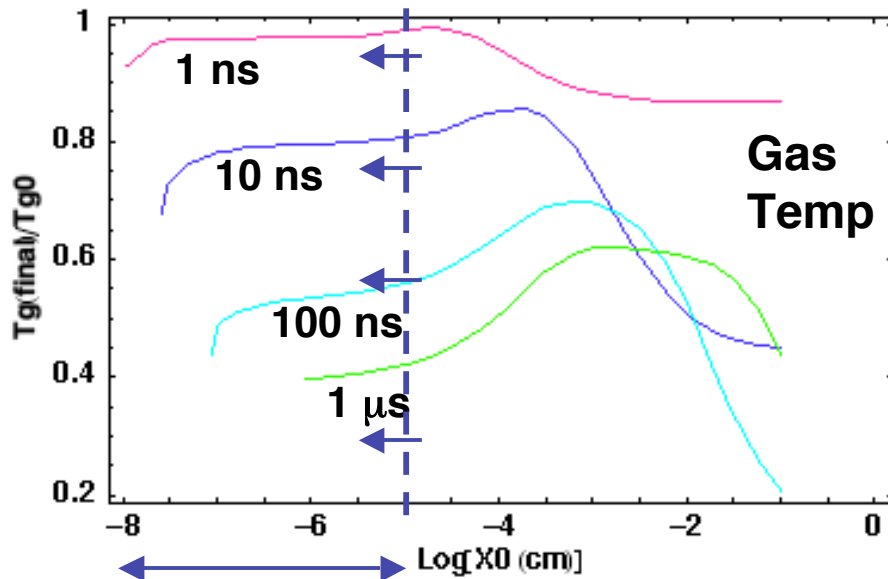
Assumptions: $\alpha=0.5, \beta=0.5$;

$$\text{at } t=0: \quad V_{g0} = V_{l0} = \frac{4\pi X_0^3}{3}; \quad T_{g0} = T_{l0} = 10000\text{K}$$

Importance of the thermalization from liquid to gas



At long times, for droplets
In the reference case,
thermalization
Is efficient: $T_l = T_g$



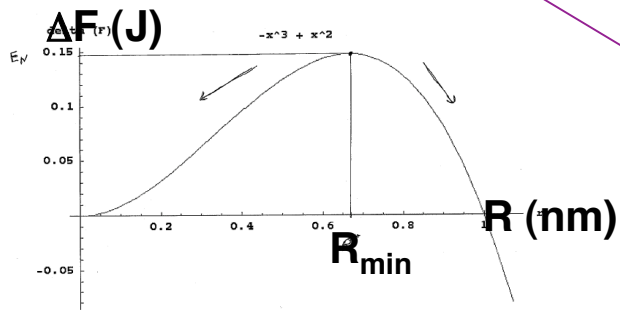
Reference case

2. Debris initially at high T and solid density: initially material is vaporized and cools adiabatically

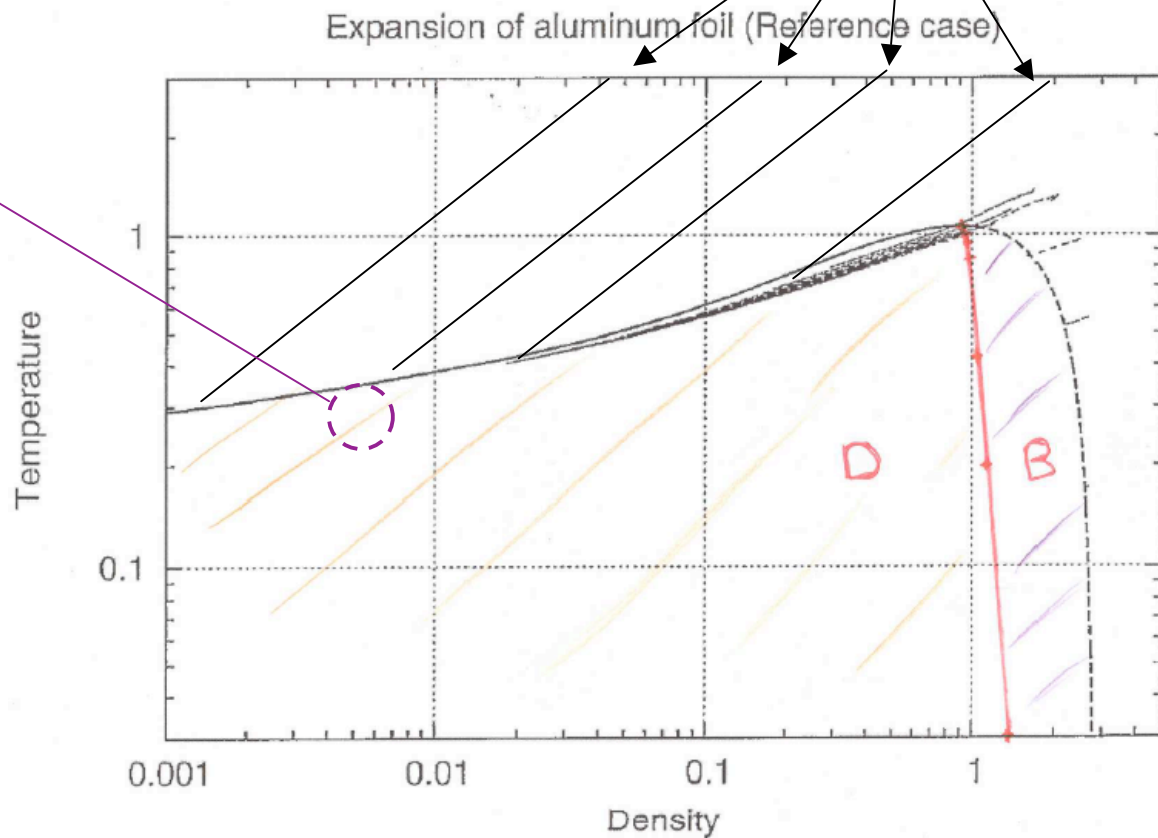
Adiabatic expansion:

$$P = nkT = P_o(\rho/\rho_o)^\gamma \Rightarrow T/T_o = (\rho/\rho_o)^{\gamma-1} \propto \rho^{2/3}$$

Nucleation of droplets?



Standard nucleation theory ($R_{min} = 2\sigma/\Delta P$) is included in the model via Kelvin's equation



Conclusion

- **Criteria for max droplet sizes will need to be compared to observations (this study is only theoretical for the moment)**
- **Model equations can be used in several different situations: high / low initial temperature, 1-D / 3-D expansion of the cell (3-D when the distance travelled becomes \sim spot radius)**
- **This study gives tools that should help to understand the upcoming WDM foil heating and other ICF experiments (debris problems)**

References

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- [4]: J. M. Rallison, The deformation of small viscous drops and bubbles in shear flows, *Annual Review of Fluid Mechanics*, 16, 45-66, 1984
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