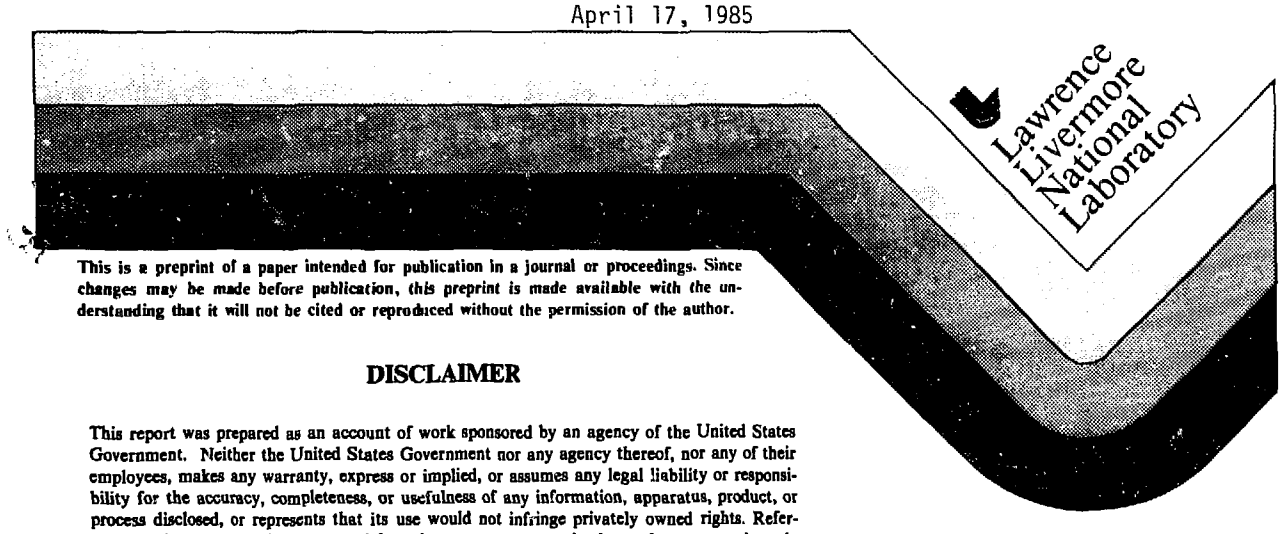
UCRL- 91954 Rev. 1
PREPRINT
CONF-850310--87

Fragmentation of Suddenly Heated Liquids in ICF Reactors

James A. Blink
William G. Hoover

This paper was prepared for submittal to the 6th ANS Topical Meeting on Technology of Fusion Energy, San Francisco, CA March 3-7, 1985.

April 17, 1985



FRAGMENTATION OF SUDDENLY HEATED LIQUIDS IN ICF REACTORS*

JAMES A. BLINK AND WILLIAM G. HODVER
Lawrence Livermore National Laboratory and
University of California at Livermore-Davis
P. O. Box 5508, L-487
Livermore, California 94550
(415) 422-8258

UCRL--91954-Rev.1

DE85 010934

ABSTRACT

Fragmentation of free liquids in Inertial Confinement Fusion reactors could determine the upper bound on reactor pulse rate because increased surface area will enhance the cooling and condensation of coolant ablated by the fusion x rays. Relaxation from the suddenly (neutron) heated state will move a liquid into the negative pressure region under the liquid-vapor P-V dome. The resulting expansion in a diverging geometry will hydrodynamically force the liquid to fragment, with vapor then forming from the new surfaces to fill the cavities. An energy minimization model is used to determine the fragment size that produces the least amount of non-fragment-center-of-mass energy; i.e., the sum of the surface and dilational kinetic energies. This model predicts fragmentation dependence on original system size and amount of isochoric heating as well as liquid density, Grüneisen parameter, surface tension, and sound speed. A two dimensional molecular dynamics code was developed to test the model at a microscopic scale for the Lennard-Jones fluid with its two adjustable constants chosen to represent lithium. The numerical experiments produced reasonable agreement with the model. Considerable fragmentation is predicted in the high energy density HYLIFE reactor, with minimum fragmentation in other (low energy density) reactors.

INTRODUCTION

In several inertial confinement fusion (ICF) reactor concepts, the fusion neutrons are suddenly deposited into liquid metals having free surfaces within the vacuum chamber. The neutron energy deposition is so fast that the liquid has little opportunity to expand during the deposition time; hence, the deposition is effectively at constant volume, or isochoric. In this study, energy deposition is considered "isochoric" if the deposition time is less than the sound wave transit time of the liquid region. The suddenly increased temperature and energy content of the liquid produces a sudden increase in pressure. Since the free surfaces are exposed to effectively zero pressure, tensile relief waves propagate inward. Tension eventually causes liquids to cavitate, leading to fragmentation in liquids with available expansion volume. The fragments have velocities due to acceleration by the pressure difference across the tensile wave.

Liquid metal fragmentation has two impacts on ICF reactor design. First, the fragments eventually collide with the structure, causing a pressure load which can be estimated from average fragment velocities predicted by continuum mechanics computer codes. (However, fragment velocity distributions could cause an additional erosion problem from the higher-than-average-velocity fragments). Second, the fragment size determines the liquid surface area available to interact thermally with superheated gas or plasma produced by the absorption of the short-ranged fusion x rays and debris. Since the cooling and condensation times depend on the cooling surface area, it is possible that the maximum chamber pulse rate will be set by the degree of fragmentation.

In this article, which summarizes a Ph.D. thesis[1], rapid vaporization is considered and rejected as a driving mechanism for fragmentation of liquid lithium in ICF reactors. An energy minimization model of liquid fragmentation is developed. Because the model does not consider the dynamic process of fragmentation, numerical experiments are used to study the fragmentation dynamics and to test the

*Work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. W-7405-ENG-48.

jsw

predictions of the model. These experiments use the technique of molecular dynamics to follow the evolution of up to several thousand liquid atoms following sudden heating. For simplicity, and to better model the quasi-two-dimensional expansion of an ICF reactor jet column, the numerical experiments are performed in two dimensions using the Lennard-Jones "6-12" interatomic potential.

ISOCHORIC NEUTRON HEATING IN ICF REACTORS

Neutron transport computer codes have been used to calculate the time and space dependent neutron energy deposition levels in several ICF reactors. For example, the neutron energy deposition time in the HYLIFE[2] reactor* is ~ 0.1 to 1 μs. The time for relief of the induced pressure is the liquid thickness (or diameter) divided by the sound speed. The sound speeds, c, of lithium and $Li_{17}Pb_{83}$ are 4500 and 1800 m/s. The heating is "isochoric" if 2R/c > 0.1 μsec. That is, for isochoric heating, the minimum radius of the liquid is 0.25 mm for lithium and 0.1 mm for $Li_{17}Pb_{83}$. This condition is satisfied in several ICF reactors, including HYLIFE. The pressure rise from the suddenly added neutron energy can be calculated from the Grüneisen equation of state, $\Delta P = \rho_m \Gamma e$, where e is the specific energy deposited in J/kg, Γ is the Grüneisen parameter (1.0 for lithium, 2.0 for $Li_{17}Pb_{83}$), and ρ_m is the mass density (485 and 9320 kg/m^3, respectively). For HYLIFE, the peak neutron induced pressure is ~ 400 MPa or 4 kbar. The jump-off velocity, v_s, of the expanding liquid can be calculated by considering the pressure drop across a moving rarefaction wave. The momentum conservation equation is $\Delta P = \rho_m c v_s$. The jump-off velocity for HYLIFE is ~ 174 m/s.

SUDDEN VAPORIZATION AS A FRAGMENTATION MECHANISM

Relaxation from the suddenly heated state will move a liquid into the negative pressure region under the liquid-vapor P-V dome. In this section, the consequent vaporization is examined to determine if it is fast enough and energetic enough to drive the fragmentation process. The lithium equation of state developed by Young[3] was used to determine the paths followed on a P-V diagram following sudden heating of lithium in the HYLIFE reactor (Fig. 1). The initial condition is on

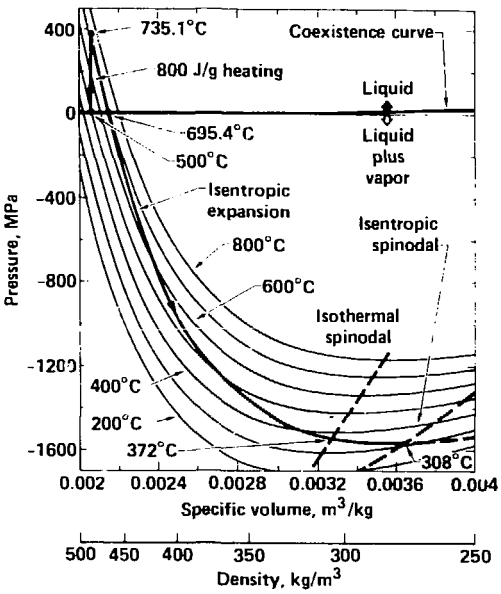


Fig. 1. P-V diagram of the heating and expansion of a lithium jet. Due to the restricted specific volume range of the diagram, the coexistence curve appears to be flat at zero pressure. The critical pressure of 114 MPa is at 0.011 m^3/kg (not shown). The dashed isothermal and isentropic spinodal lines cross the low right corner. The "two-phase" isotherms are analytic continuations of the single phase isotherms.

the saturated liquid line at 500°C (485 kg/m^3). The fusion neutrons isochorically add a maximum of 800 kJ/kg. The liquid temperature and pressure quickly rise to 735°C and 380 MPa with no density change. As the relief wave moves into the jet, an adiabatic (isentropic) expansion begins. During expansion to the saturation line (and Γ ~ 0), the liquid temperature falls to 695°C, and the internal energy falls by ~ 16 kJ/kg. Use of the 174 m/s jump-off velocity shows that 15.2 kJ/kg of kinetic energy is produced by the tensile wave, without considering any phase change. Hence, most of the "lost" internal energy is converted to kinetic energy.

The expansion continues into the two phase liquid-vapor region until phase separation returns the fluid to the saturated liquid and vapor lines. When the isentrope is analytically continued into the two phase region, negative pressures are indicated. The isentrope is not continued beyond the spinodal line (where it has zero slope) since the fluid

*HYLIFE has 175 free falling, 20-cm diameter lithium jets in an array around the fusion source. It is used as an example in this article because it has a higher neutron heating level, ~ 800 kJ/kg, than most ICF reactors, and thus should fragment more extensively.

is then unstable to phase separation back to the spinodal, probably on a sub-nanosecond time scale. Between the coexistence curve and the spinodal, the fluid is metastable, and it eventually separates into saturated liquid and vapor phases (on the coexistence curve) by the sequential processes of nucleation and growth in the bulk liquid or by vaporization from the new free surfaces.

If the isentropic expansion continues all the way to the spinodal, the specific volume would increase by 50% and the vapor volume would be ~ 0.001 m^3/kg-liquid. If the vapor were in equilibrium with 735°C liquid, the vapor pressure would be ~ 120 Pa (0.9 torr) and the vapor specific volume ~ 9690 m^3/kg-vapor. The quotient of the two specific volumes is 100 μg-vapor per kg-liquid, an extremely low vaporization fraction. Since vaporization requires 20.7 MJ/kg-vapor, only 2.1 J/kg-liquid are required for vaporization. This is about 7000 times less energy than the kinetic energy produced by the hydrodynamic expansion. Thus, the energy balance indicates that sudden vaporization (by spinodal decomposition) cannot be the driving force for the hydrodynamic expansion and fragmentation.

It is unlikely that the spinodal line would be reached in a liquid lithium inertial fusion reactor. At the spinode, the liquid tension is ~ 1500 MPa, much larger than the tensile strength of solid lithium or the tension induced in extremely clean water during carefully controlled experiments. In an ICF reactor, the entrained gas, target debris, and corrosion products provide an abundance of potential nucleation sites, allowing a more gradual phase change by the processes of nucleation and growth. However, vapor bubble growth times (milliseconds) are longer than the liquid's expansion time (80 μs for a 50% volume increase in HYLIFE); thus vapor growth is also too slow to drive the fragmentation. Instead, the voids created by fragmentation must equilibrate by filling with vapor from the new free surfaces.

THE ENERGY MINIMIZATION MODEL

The model minimizes the sum of the surface energy density and the fragment non-translational kinetic energy density as a function of fragment size. Since the fragment translational kinetic energy is much larger than the non-translational (dilational) kinetic energy, this model predicts much larger fragments than simpler models which require the surface forces to balance either the sudden pressurization or the resulting dynamic pressure ($\rho v_s^2/2$). For example, in HYLIFE, the two simple models predict fragment radii of 1.8 and 90 nm, respectively, while the energy minimization model predicts 2.1 mm.

The energy minimization process, which is similar to the Griffith Theory of Fracture[4] familiar to material scientists, was first proposed by Grady[5] and extended by Glenn[6]. Fragment size, a, is used as the independent variable, and the kinetic energy is divided into the motion of the fragment center of mass and the fragment dilation. The dilational kinetic energy is added to the surface energy, and the sum is minimized with respect to the fragment size. The velocity divergence, $\nabla\cdot\vec{v} = -\dot{\rho}/\rho$, was the independent variable in Grady's result,

$$a = \left[\frac{(D+2)D^2\gamma}{(\dot{\rho}/\rho)^2}\right]^{1/3} \qquad (1)$$

where D is the number of dimensions (2 or 3) and γ is the surface tension (0.35 J/m^2 for lithium and 0.435 J/m^2 for $Li_{17}Pb_{83}$). This result requires assumption of a homogeneous expansion, i.e., constant velocity divergence. Grady successfully compared his result to oil shale fragmentation and breakup of explosively loaded pipes.

Glenn[6] carried out a series of hydrodynamic calculations of isochorically loaded spheres in which tensile fragmentation was not allowed. The resulting velocity profiles were quite flat for r/R > 0.1, and the velocity divergence profiles were even flatter. Hence, for most of the liquid mass, the velocity divergence is roughly constant (Dv_s/R) where R is the initial system radius. Then

$$a = \left[\frac{D+2}{\rho_m}\gamma\left(\frac{Rc}{Re}\right)^2\right]^{1/3} \qquad (2)$$

where e is the isochoric heating per unit mass.

If the sphere size is chosen to avoid fragmentation (a=R), this formula agrees well with the two simpler models because all the kinetic energy is dilational. For example, with HYLIFE loading, the stable (when a=R) drop size prediction is 114 nm compared to 1.8 and 90 nm from the simple models. Thus, the jump-off velocity gives a much better estimate of the available energy for surface formation than does the total added energy. Further, if fragmentation is extensive, only a small fraction of the jumpoff kinetic energy is balanced against the increased surface energy; the larger fraction becomes translational energy of the fragments.

The Grady-Glenn derivation was extended[1] to include the velocity divergence as a function of radial position within the original drop rather than a single value. The fragments near the drop center will be up to

an order of magnitude smaller and the outermost fragments will be up to 31% larger than the prediction based on constant velocity divergence. Even after this correction, the model still assumes local homogeneity within the fragment. Hence, for large fragment size (a approaching R), the model continues to br ' down because the volocity divergence is not constant within the fragment.

Table 1 shows the predicted fragment sizes from Eq. 2 for several ICF reactors. The table also shows that the fragment dilational kinetic energy is small compared to the translational energy. The low energy density reactor concepts are predicted to have little or no fragmentation. For the high energy density HYLIFE inner jets, the model predicts fragment diameters of ~ 1% of the jet diameter. The overall HYLIFE fragmentation will increase the liquid surface area by about two orders of magnitude during the period that the hot gas caused by ablation blows through the jet array (60-300 μs after the fusion pulse). After the hot gas blows through the fragmenting array, the fragment translational energy distribution (higher velocities for the fragments from the inner jets) causes the fragments to coalesce at several ms after the pulse. Then, the coalesced liquid again fragments due to its uniform motion in a diverging geometry. The fragment size distribution during this later period determines the condensation rate, at least until homogeneous nucleation begins. The fragment size distribution during the period the gas transits the array influences the early stages of gas cooling and the structural load imposed when the gas reaches the wall.

MOLECULAR DYNAMICS VALIDATION OF THE MODEL

The development of the Grady-Glenn model was very exciting because it gave intuitively reasonable estimates of fragment size. However, the model is too simple in that it only determines the lowest final energy state and it only considers spherical or circular fragments. Hence, a series of molecular dynamics experiments were carried out to test the model's ability to predict fragment size as a function of system size and isochoric heating level. These calculations are summarized in Ref. 11 and described in detail in Ref. 1; in this report, only the results are presented.

Molecular dynamics calculations were carried out on two dimensional circular liquid regions containing 169, 721, 2611, or 14491 atoms. These liquid regions were equilibrated at a constant density within a confining wall at various temperatures between saturation and an energy level above that of HYLIFE, and then released. During the subsequent fragmentation, the translational, rotational, thermal, and potential energies and the population were monitored for each fragment.

The fragment sizes (in atoms) from two 2611 atoms runs are shown in Fig. 2. In each case, the raw data have been slightly adjusted (using the Grady-Glenn energy minimization

Table 1. Predicted fragmentation in several ICF reactors. The fragmentation was calculated from the formula for unconstrained spheres.

Reactor	Fluid	Thick. (cm)	Fragm. Diam. (cm)	Suddenly added specific energy (J/kg)	Transl. specific kinetic energy (J/kg)	Dilational specific kinetic energy (J/kg)
HYLIFE[2] inner jet	Li	20	0.21	800,000	15,800	1
HYLIFE outer jet	Li	20	1.3	50,000	61.6	0.16
HIBALL[7] (inner jet, ignoring SiC sock)	LiPb	3	1.8	500	0.14	0.013
Modified Wetted Wall ††,[8]	Li	4	2.7	3500	0.22	0.081
EAGLE[9]	Li	0.05	0.14†	3700	0†	0.34†
Pulse*Star[10]	LiPb	1	0.53	1000	0.58	0.042

† No breakup predicted by the energy minimization model.
†† Liquid motion is not in diverging geometry.

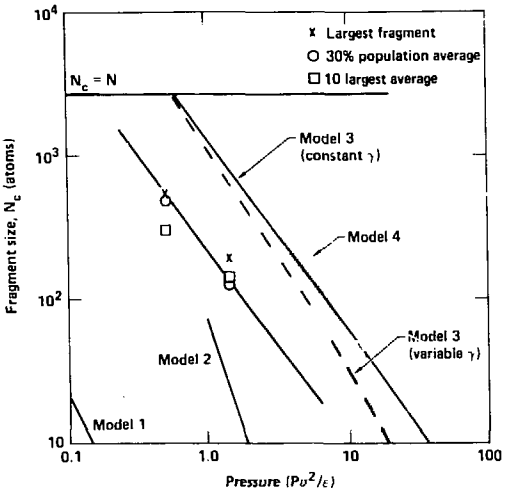


Fig. 2. Observed and predicted fragment sizes (atoms) as a function of initial pressure, for two 2611 atom runs. The data and model predictions have been slightly adjusted to constant initial conditions. The three observed values for each run are for the largest fragment, the average of the ten largest fragments, and the average of the largest fragments comprising 30% of the system population (less monomers). Model 4 is model 3 with only the kinetic energy in an outer shell being used to balance the surface energy.

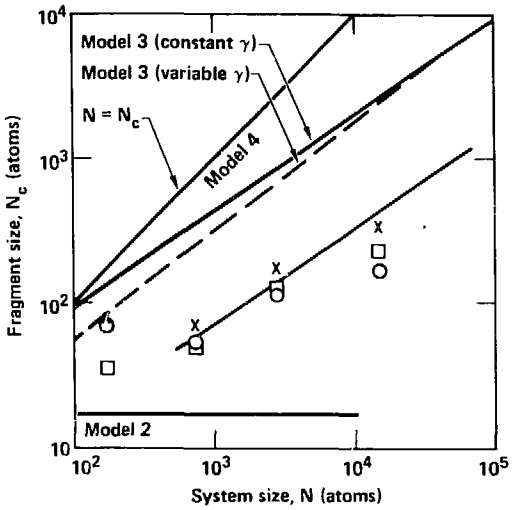


Fig. 3. Observed and predicted fragment sizes (atoms) as a function of system size, for similar heating levels. The nomenclature is identical to that of Fig. 2. The model 1 slope is also zero, but below the lower limit of this graph.

model, "model 3") to uniform initial conditions (2611 non-monomer atoms and a specified density, sound speed, and surface tension). The only remaining variable in the model is the initial pressure. The slopes of the data (presented three ways) are -1.03, -0.86, and -1.42, respectively, these values bracket the predicted slope of -4/3 from model 3 reasonably well. To illustrate the sensitivity of the fragmentation to fragment-size dependent surface tension, the model 3 prediction curve is also shown using the lower surface tensions at the actual fragment sizes; the "observed" data would be similarly steeper when the surface tension correction is eliminated. Finally, the predictions from 3 other models are shown; clearly, only model 3 (the Grady-Glenn model) has the correct dependence on isochoric heating level.

The fragment sizes from the highest pressure run for each system size (14491, 2611, 721, and 169 atoms) are shown in Fig. 3. The nomenclature is identical to that of the previous figure. The data were again slightly adjusted to uniform initial conditions (in pressure, density, sound speed, and surface tension). The only remaining variable in the models is the system size (total number of particles), N. The slopes of the middle sections of the three fragment size data sets are 0.75, 0.69, and 0.64, respectively. These observed values bracket the predicted slope of 2/3 from model 3. The 169 atom data were not used to compute the slope because of minimal fragmentation. The 14491 atom fragment sizes are probably a bit low due to a sloshing motion present in the system at the time the confining boundary was removed. However, if the slopes are computed using line segments between the 721 and 14491 data sets, the results are 0.54, 0.50, and 0.41, respectively. Thus, the molecular dynamics results indicate a system size dependence of the 2/3 power (the illustrated line), but support that slope with an uncertainty of ±0.15. This result again is consistent with the energy minimization model (model 3) and inconsistent with the other models.

Although the data in Figs. 2 and 3 support the energy minimization model's power law dependence of fragment size on system size and isochoric heating level (initial pressure), the magnitudes of the observed sizes (in atoms) are about ten times lower than the model 3 prediction. Laboratory scale experiments will be needed to determine if

this is an effect of the small system size, or if it extends to experiment and reactor sizes.

SUMMARY

The numerical experiments produced reasonable agreement with the energy minimization model. The qualitative dependences of fragment size on system size and heating level were correct, and the larger fragment sizes were within an order of magnitude of the predictions. Thus, it is concluded that the Grady-Glenn model is a useful tool for ICF reactor design. The model predicts significant fragmentation only in high-energy-density reactors like HYLIFE; low-energy-density designs like Pulse*Star and EAGLE will be required to provide adequate droplet surface area by means other than the hydrodynamic response to the fusion neutron pulses.

REFERENCES

1. J. A. BLINK, "Fragmentation of Suddenly Heated Liquids," Ph.D. Thesis, University of California at Davis/Livermore (Dec. 1984). Also available as LLNL report UCRL-53604.

2. M. J. MONSLER, J. HOVINGH, D. L. COOK, T. G. FRANK and G. A. MOSES, "An Overview of Inertial Fusion Reactor Design," Nucl. Technol./Fusion, 1, p. 3-2, Sec. IX, (1982). See also Lawrence Livermore National Laboratory Laser Program Annual Reports for 1978, 1979, 1980, and 1981 (UCRL-50021-year, where "year" is '78, '79, '80, or 81).

3. D. A. YOUNG, "A Soft-Sphere Model for Liquid Metals," Lawrence Livermore National Laboratory Report UCRL-52352 (1977).

4. F. A. McCLINTOCK and A. S. ARGON, editors, Mechanical Behavior of Materials, Addison-Wesley Publ. Co., Reading, Mass., p. 489 (1966).

5. D. E. GRADY, "Local Inertial Effects in Dynamic Fragmentation," J. Appl. Phys., 53, 1, p. 322 (1982).

6. L. A. GLENN, "On the Fragmentation of Condensed Material by Isochoric Heating and Release," Lawrence Livermore National Laboratory Report UCID-19737 (1983).

7. B. BADGER, et al., "HIBALL-A Conceptual Heavy Ion Beam Driven Fusion Reactor Study," University of Wisconsin Report UWFDM-450 (1981).

8. J. H. PENDERGRASS, T. G. FRANK and I. O. BOHACHEVSKY, "A Modified Wetted-Wall Inertial Fusion Reactor Concept," Proceedings of the 4th Topl. Mtg. Technology of Controlled Nuclear Fusion, King of Prussia, Penn., p. 1131 (1981).

9. W. O. ALLEN, et al, "Phase I: Engineering Test Reactor Goal Specification Final Report," Electric Power Research Institute Report EPRI-1527 (1982).

10. J. A. BLINK and N. J. HOFFMAN, "Tritium Control and Activation in the Pulse*Star Reactor," Proceedings of the IEEE 10th Symposium on Fusion Engineering, Philadelphia, Penn. (1983).

11. J. A. BLINK and W. G. HOOVER, "Fragmentation of Suddenly Heated Liquids," submitted to Phys. Rev. A. Also available as LLNL report UCRL-91954.