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TITLE: THREE-DIMENSIONAL MODELING OF SHOCK INITIATION OF HETEROGENEOUS EXPLOSIVES

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THREE-DIMENSIONAL MODELING OF SHOCK INITIATION OF HETEROGENEOUS EXPLOSIVES

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ABSTRACT

The basic processes in the shock initiation of heterogeneous explosives have been investigated theoretically using a model of a cube of nitromethane containing 91 cubic air holes. The interaction of a shock wave with the density discontinuities, the resulting hot spot formation and interaction, and the buildup to propagating detonation were computed using three-dimensional numerical Eulerian hydrodynamics with Arrhenius chemical reaction and accurate equations of state.

The basic process in the desensitization of a heterogeneous explosive by preshocking with a shock pressure too low to cause propagating detonation was numerically modeled.

Introduction

The hydrodynamic stability of one-dimensional detonations in an ideal gas of constant heat capacity undergoing an exothermic, irreversible, unimolecular reaction with an Arrhenius-law temperature dependence has been studied analytically by Erpenbeck.[1] The analysis gives no information about the nature of the time-dependent behavior of the flow for finite perturbations (the stability) of the ideal gas reaction zone using a one-dimensional characteristic method. In those cases for which Erpenbeck's linearized analysis has shown the steady-state solution to be unstable to infinitesimal longitudinal perturbations, flows started in a configuration approximating the steady-state solution exhibited nondecaying oscillations; in those cases for which Erpenbeck's analysis showed the steady-state solution to be stable, perturbations were found to decay.[2]

In Reference 3 we described the results of our studies of the time-dependent behavior of the flow (the stability) of the ideal gas, nitromethane and liquid TNT reaction zones to finite longitudinal and transverse perturbations using finite difference methods to solve the reactive Navier-Stokes equations of fluid dynamics. We also described the time-dependent behavior of the flow of stable overdriven nitromethane detonations formed by pistons of various configurations.

The constant velocity piston calculations with a resolved reaction zone show details of the process of shock initiation of nitromethane. The basic features are identical to those of the flow computed with an unresolved reaction zone.[4] The shocked nitromethane first completely decomposes at the piston and achieves a detonation with a peak pressure that builds up toward the C-J pressure of the high density shocked nitromethane. The detonation wave overtakes the shock wave and the pressure at the end of the reaction zone decays toward the piston pressure.

If one introduces gas bubbles or grit into a homogeneous explosive such as a liquid or a single crystal, thereby producing a heterogeneous explosive, the minimum shock pressure necessary to initiate propagating detonation can be decreased by one order of magnitude.

Heterogeneous explosives, such as PBX 9404 or Composition B, show a different behavior than homogeneous explosives when propagating along confining surfaces. A heterogeneous explosive can turn sharp corners and propagate outward, and depending upon its sensitivity, it may show either very little or much curvature when propagating along a metal surface. The mechanism of initiation for heterogeneous explosives is different than the simple Arrhenius kinetic model found adequate for homogeneous explosives. Heterogeneous explosives are initiated and may propagate by the process of shock interaction with density discontinuities such as voids. These interactions result in hot regions that decompose and produce increasing pressures that cause more and hotter decomposing regions. The shock wave increases in strength, releasing more and more energy, until it becomes strong enough that all of the explosive reacts and detonation begins.

The numerical modeling of the interaction of a shock wave with a single density discontinuity was reported in Reference 5 where an 8.5-GPa shock interacting with a single spherical hole in nitromethane was studied.

The study was extended to four rectangular holes[5] where it was determined that a 0.0032-mm-radius cylindrical void would initiate propagating detonation and a 0.001-mm-radius void would form a hot spot which failed to propagate because of rarefactions cooling the reactive wave.

We have studied the buildup of an 8.5-GPa shock wave in nitromethane as it interacts with 91 cubes, 0.002 mm or 0.0004 mm on a side. The cubes simulate a random spacing.

It has been observed that preshocking a heterogeneous explosive with a shock pressure too low to cause propagating detonation in the time of interest can cause a propagating detonation in unshocked explosive to fail to continue propagating when the detonation front arrives at the previously shocked explosive. For explosives that have been previously shocked, it has been experimentally observed[6] that the distance of run to detonation for several multiple-shocked explosives is determined primarily by the distance after the second shock has overtaken the lower pressure shock wave (the preshock). In this study we examine the basic process in the desensitization of heterogeneous explosives by preshocking.

Computational Method

The three-dimensional Eulerian reactive hydrodynamic code 3DE is described in Reference 7. It uses techniques identical to those described in detail in Reference 5 and used successfully for describing two-dimensional Eulerian flow with mixed cells and multicomponent equations of state, and for modeling reactive flow.

The three-dimensional code has been used to study the interaction of two, three, and five colliding, diverging spherical detonation waves in PBX 9404. As described in Reference 8, the size and magnitude of the high-pressure double, triple, quadruple, and quintuple interactions depend upon the number and relative location of the initiators. The initiation of propagating detonation in the insensitive explosive PBX 9502 by triple shock wave interaction resulting from three initiators has also been studied.

The three-dimensional computational grid contained 28 by 28 by 28 cells, each 0.001 mm on a side. Ninety-one cubic air holes, each 0.002 mm on a side were placed in the grid in 4 layers of 4 holes on a side, separated by 3 layers of 3 holes on a side. The distance between hole centers in a layer was 0.006 mm and between layers the distance between hole centers was 0.005196 mm. The hole corners were offset by 0.0014 mm between layers. The initial locations of the air holes are shown in Fig. 1.

The nitromethane equations of state used were identical to those described in Reference 5. The Arrhenius rate constants used were 40 kcal/mole for activation energy and 1.27×10^8 microsecond^{-1} for the frequency factor. The detonation wave is stable at C-J velocity for an activation energy of 40 kcal/mole. The frequency factor is 100 times larger than used for nitromethane in Reference 5.

A piston was applied to the bottom of the nitromethane cube, shocking the nitromethane initially to 8.5 GPa and 1100 K. When the shock wave interacts with a hole, a hot spot with temperatures several hundred degrees hotter than the surrounding explosive is formed in the region above the hole when it is collapsed by the shock wave. The hot region decomposes and contributes energy to the shock wave which has been degraded by the hole interaction.

Whether this energy is sufficient to compensate for the loss from the hole interaction depends upon the magnitude of the initial shock wave, the hole size, and the interaction with the flow from nearest neighbor hot spots. The objective of the study was to determine the nature of this complicated interaction.

The computational time step was 2.0×10^{-5} microseconds for the 0.002-mm hole problem. The calculations were performed on the Cray computer. The computer time for calculating the 21,952 cells for 279 cycles or time steps was 1.5 hours.

Numerical Results

The interaction of an 8.5-GPa shock in a 0.028-mm cube of nitromethane with ninety-one 0.002-mm cubical holes and chemical reaction is shown in Fig. 2. The shock interacts with the first layer of holes causing hot spots upon closure of the holes, which decompose but do not result in propagating detonation in the remainder of the nitromethane. The decomposition enhances the shock wave so that, upon interaction with upper voids, hotter and larger hot spots are formed and result in shocks sufficiently strong to induce propagating detonation.

The interaction of an 8.5-GPa shock in a 0.0056-mm cube of nitromethane with ninety-one 0.0004-mm cubical holes and chemical reaction is shown in Fig. 3. The problem is identical to that of Fig. 2, except scaled by 0.2.

The hot spots form but are so small that they are quickly cooled by the side and rear rarefactions before they can decompose enough to significantly enhance the shock wave. The hot spots continue to react slowly and keep the pressure behind the shock front from decaying. This slow decomposition was observed[5] in the shock initiation of heterogeneous explosives when an explosive continued to decompose behind the shock front and even after the shock wave passed through a slab of explosive too thin to build to propagating detonation.

The interaction of a 5.5-GPa shock in a 0.028-mm cube of nitromethane with ninety-one 0.002-mm cubical holes and chemical reaction is shown in Fig. 4. The resulting hot spots are too cool (less than 900 K) to cause appreciable decomposition before the side and rear rarefactions further reduce the temperature of the hot spot.

The interaction of a 5.5-GPa shock for 0.0016 microseconds followed by an 8.5-GPa shock in a 0.028-mm cube of nitromethane with ninety-one 0.002-mm cubical holes is shown in Fig. 5. The 5.5-GPa shock wave closes the holes and makes low-temperature hot spots, which result in very little decomposition of the explosive. The following 8.5-GPa shock wave does not have holes with which to interact. The precompressed nitromethane resembles a homogeneous explosive with the second shock causing only some additional bulk shock heating. The multiple shocking also results in a lower nitromethane shock temperature than if it had been singly shocked to 8.5 GPa.

When the 8.5-GPa shock wave catches up with the 5.5-GPa shock wave it then interacts with the remaining holes, forming hot spots which decompose and support the shock wave growth until propagating detonation occurs. This models the experimentally observed behavior of the distance of run to detonation for multiple shocked explosives being determined primarily by the distance after the second shock has overtaken the preshock.

Conclusions

The process of shock initiation of heterogeneous explosives has been investigated numerically by studying the interaction of shock waves with a cube of nitromethane with 91 holes. An 8.5-GPa shock interacting with 0.002-mm holes did not result in a propagating detonation until the shock wave had arrived at the fourth layer of holes. The enhancement of the shock wave by the chemical reaction resulting from the hot spots caused by the shock interaction with the first layer of holes resulted in hotter and larger hot spots on each subsequent interaction until the shock wave became strong enough to initiate propagating detonation in the remainder of the nitromethane. Reducing the size of the holes to 0.0004 mm resulted in a sufficient amount of the explosive decomposing to compensate for the loss in energy to the flow caused by the interaction of the shock wave with the holes. The shock wave slowly grew stronger but propagating detonation did not occur in the time of the calculation.

A 5.5-GPa shock wave resulted in insufficient heating of the resulting hot spots to cause significant decomposition.

The basic process of desensitization by preshocking is a result of the holes being closed by the low-pressure initial shock wave without resulting in appreciable explosive decomposition. The higher pressure shock that arrives later does not have holes with which to interact and behaves like a shock wave in a homogeneous explosive until it catches up with the lower pressure preshock wave.

The basic processes in the shock initiation of heterogeneous explosives have been numerically modeled in three dimensions.

References

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Figure Legends

Fig. 1. The initial configuration of 91 cubical air holes in a cube of nitromethane.

Fig. 2. The cross sections for the 12th cell in the x-direction for the interaction of an 8.5-GPa shock in a 0.028-mm cube of nitromethane with ninety-one 0.002-mm cubical holes. The interval between isopycnics is 0.2 mg/mm^3 and between burn fraction is 0.2. Shows buildup to propagating detonation.

Fig. 3. The cross sections for the 12th cell in the x-direction for the interaction of an 8.5-GPa shock in a 0.0056-mm cube of nitromethane with ninety-one 0.0004-mm cubical holes. The interval between isopycnics is 0.2 mg/mm^3 and between burn fraction is 0.2. Shows the effect of hole size.

Fig. 4. The cross sections for the 12th cell in the x-direction for the interaction of a 5.5-GPa shock in a 0.028-mm cube of nitromethane with ninety-one 0.002-mm cubical holes. The interval between isopycnics is 0.2 mg/mm^3 and between burn fraction is 0.2. Shows the effect of initial pressure.

Fig. 5. The cross sections for the 12th cell in the x-direction for the interaction of a 5.5-GPa shock for 1.6×10^{-3} μs followed by an 8.5-GPa shock in a 0.028-mm cube of nitromethane with ninety-one 0.002-mm cubical holes. The interval between isopycnics is 0.2 mg/mm^3 and between burn fraction is 0.2. Shows desensitization by preshocking.

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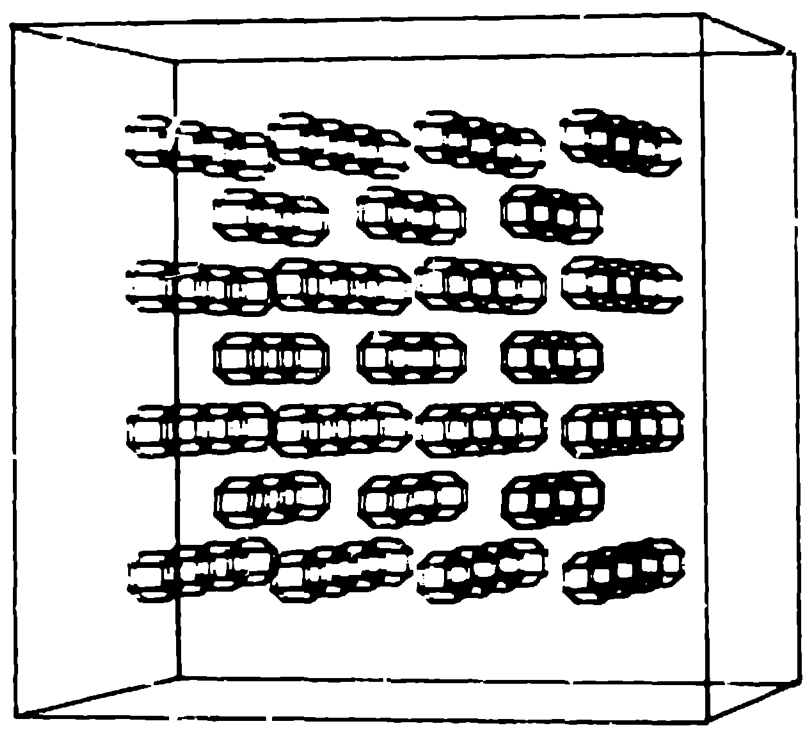
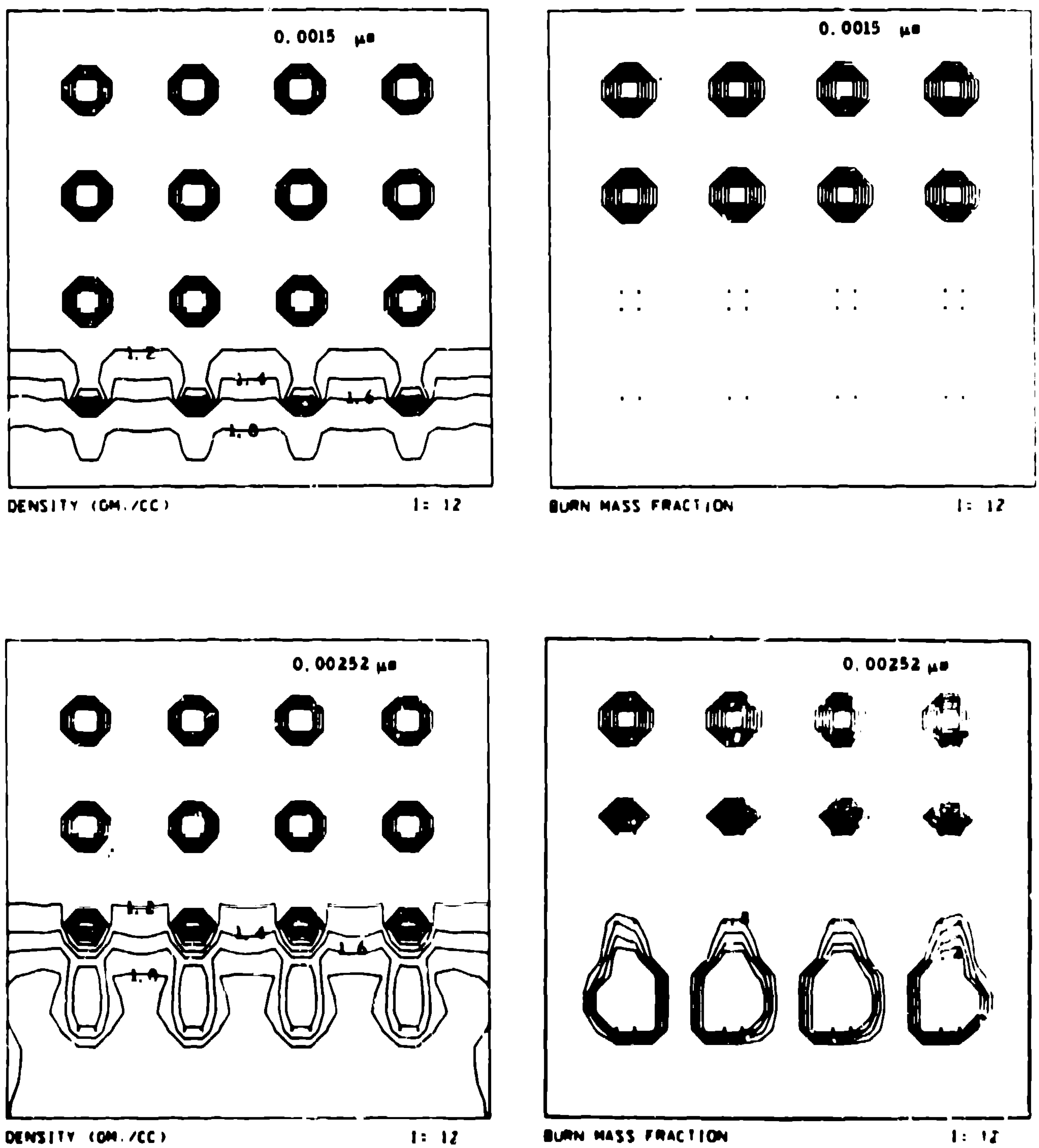
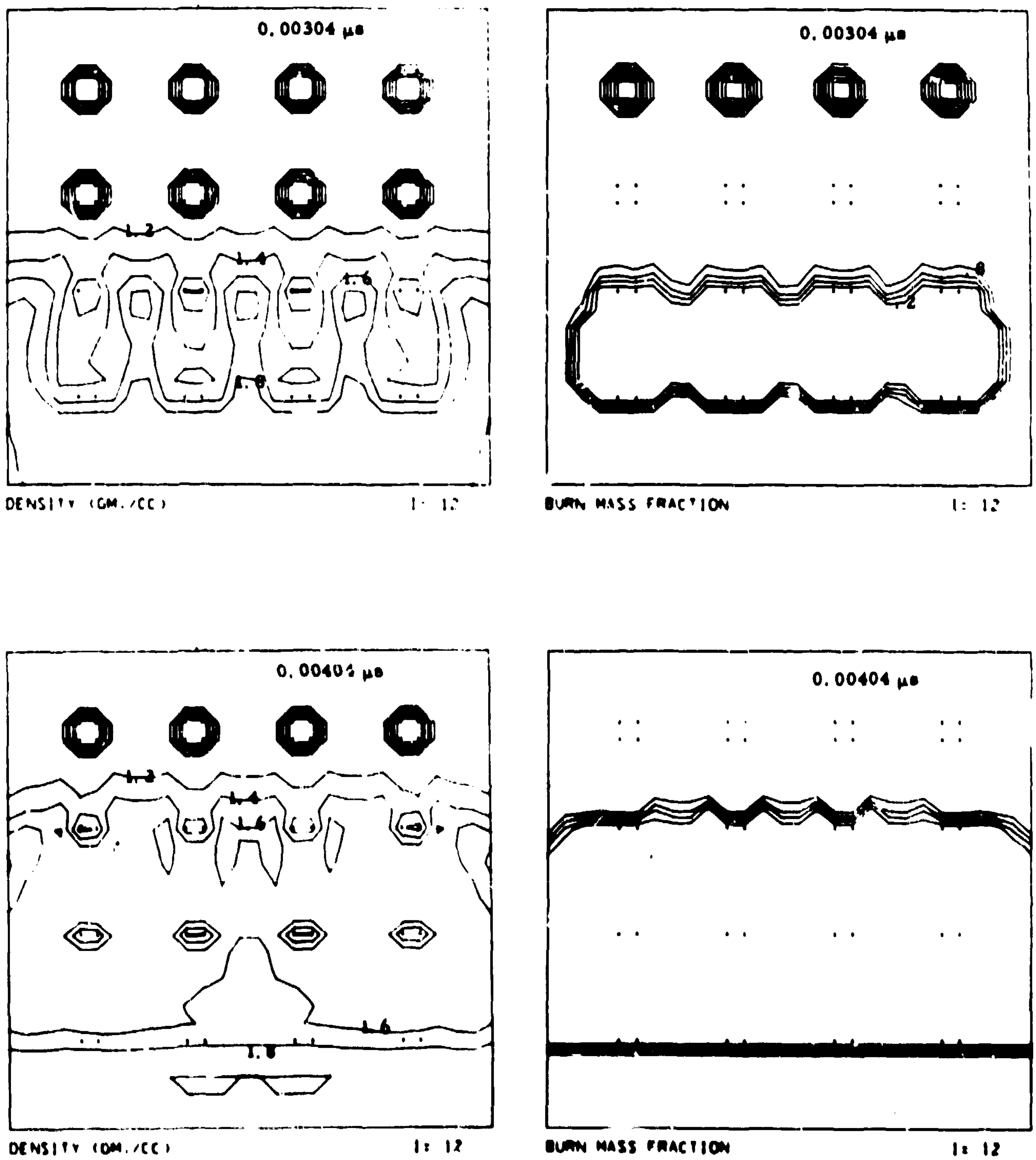


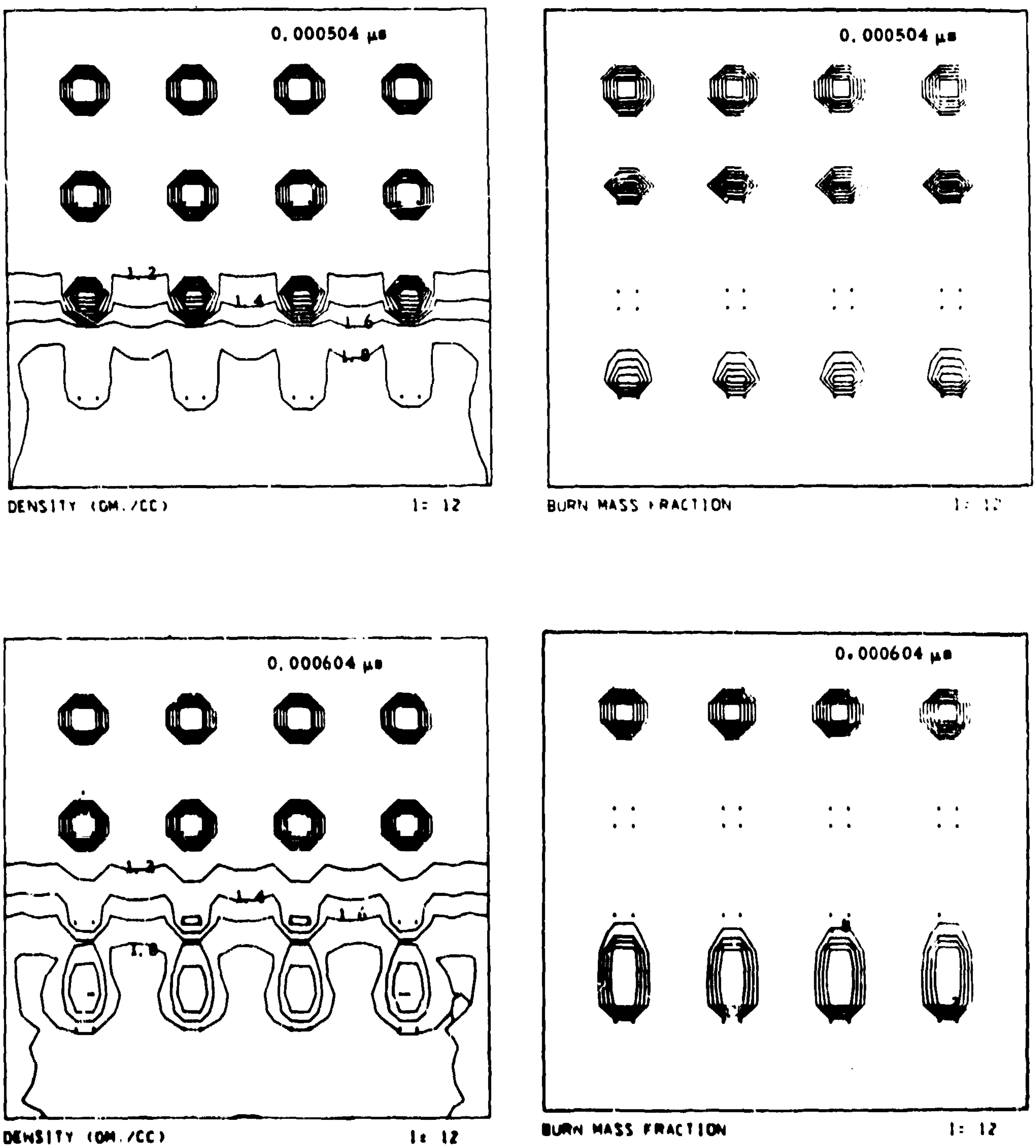
Mader - Fig. 1



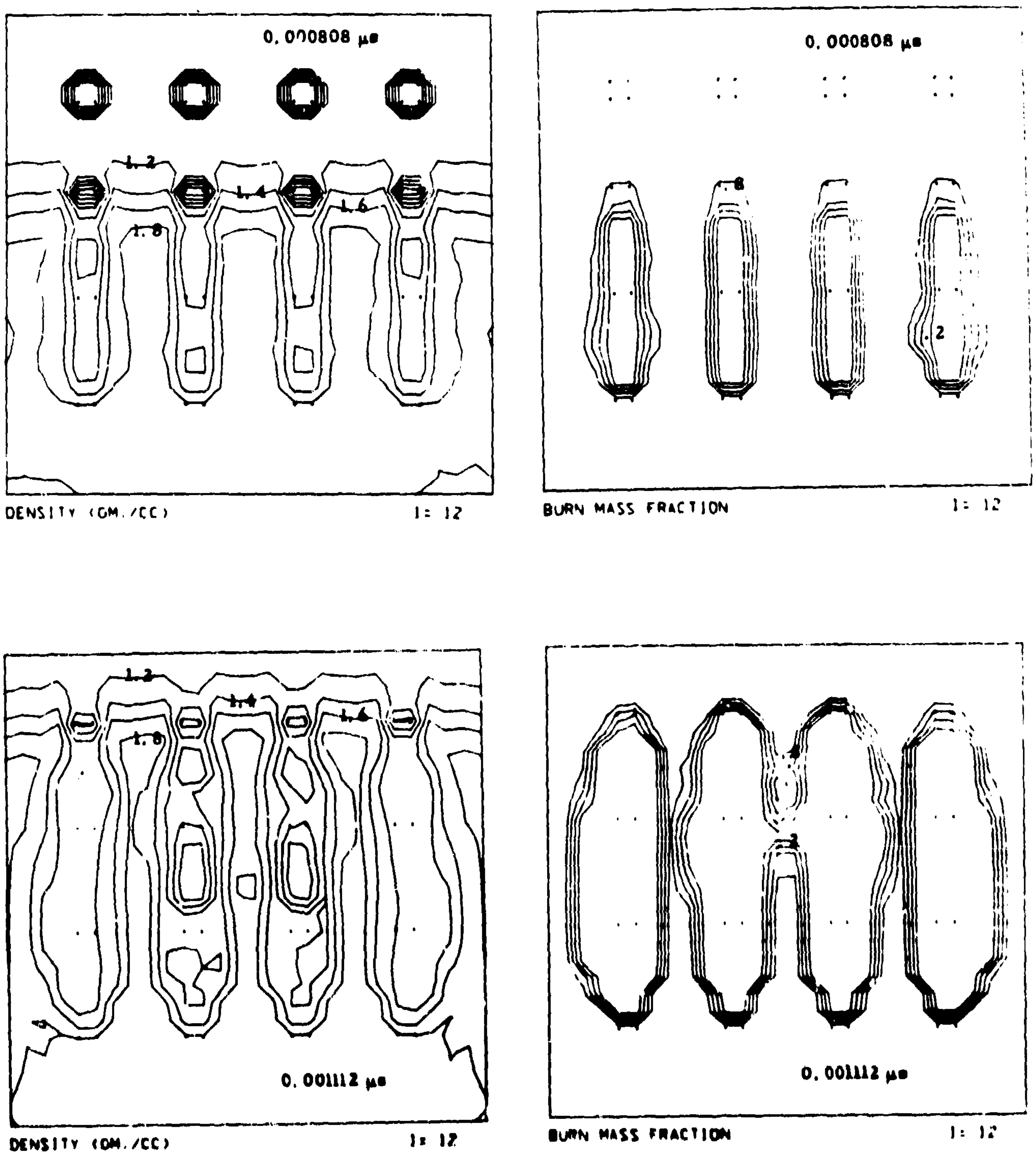
Mader - Fig. 2, p.1



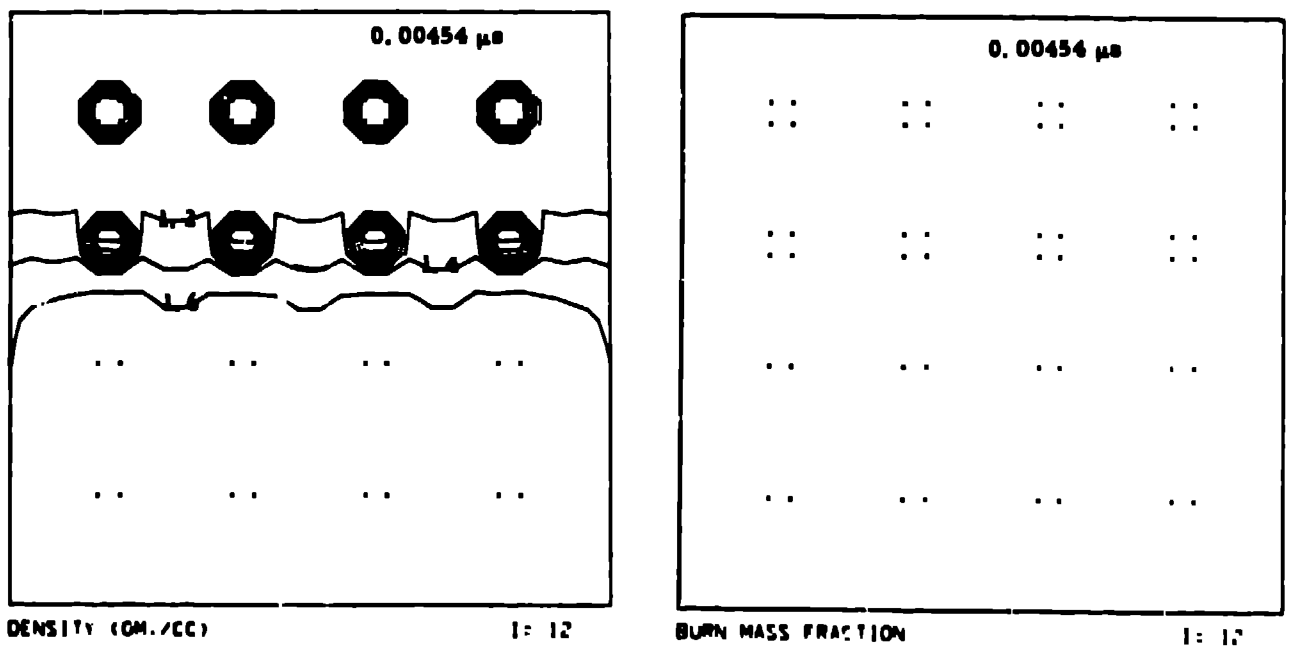
Mader - Fig. 2, p. 2



Mader - Fig. 3, p. 1



Mader - Fig. 3, p. 2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1.2
1.4
1.6
DENSITY (GM./CC)
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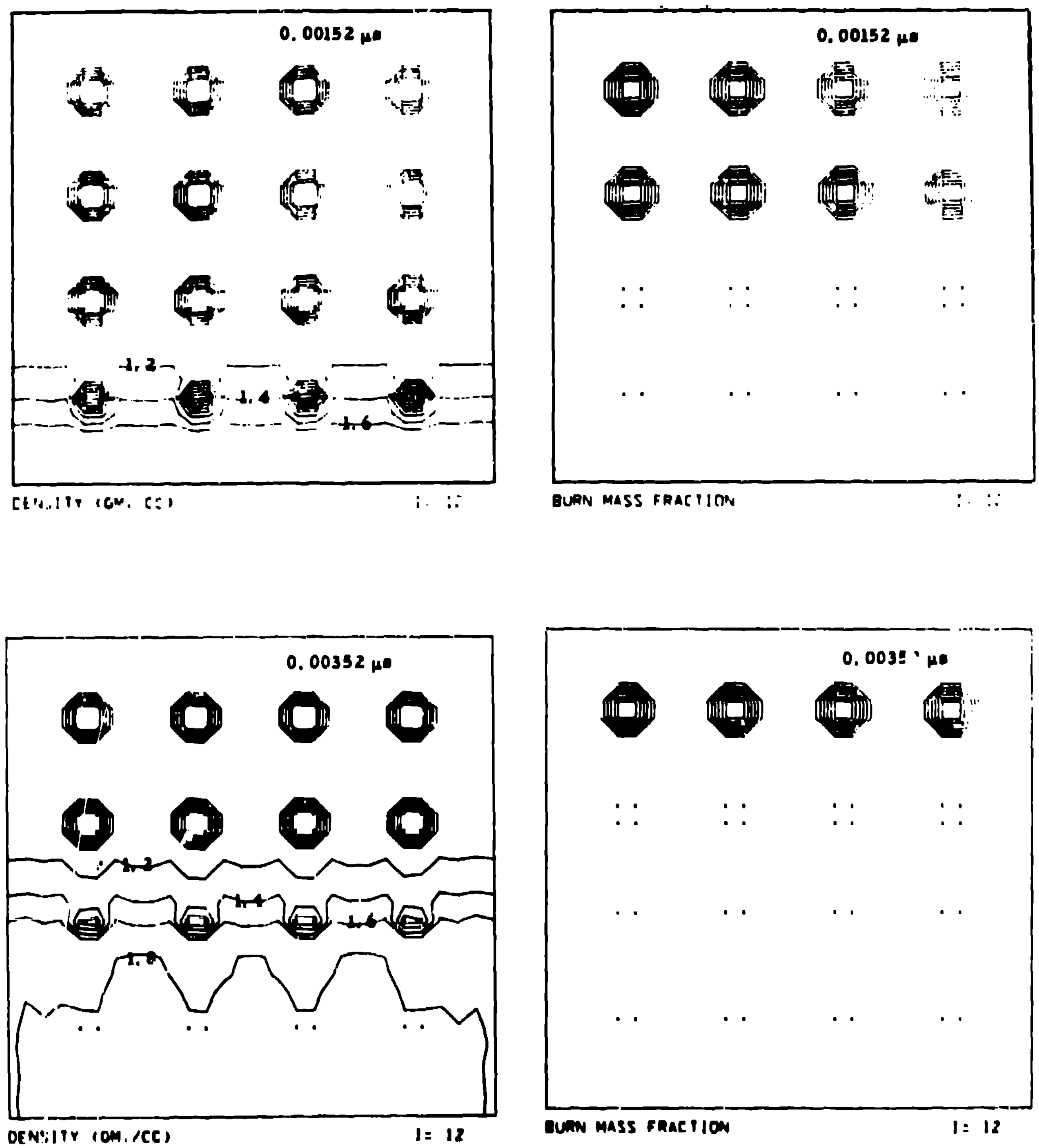
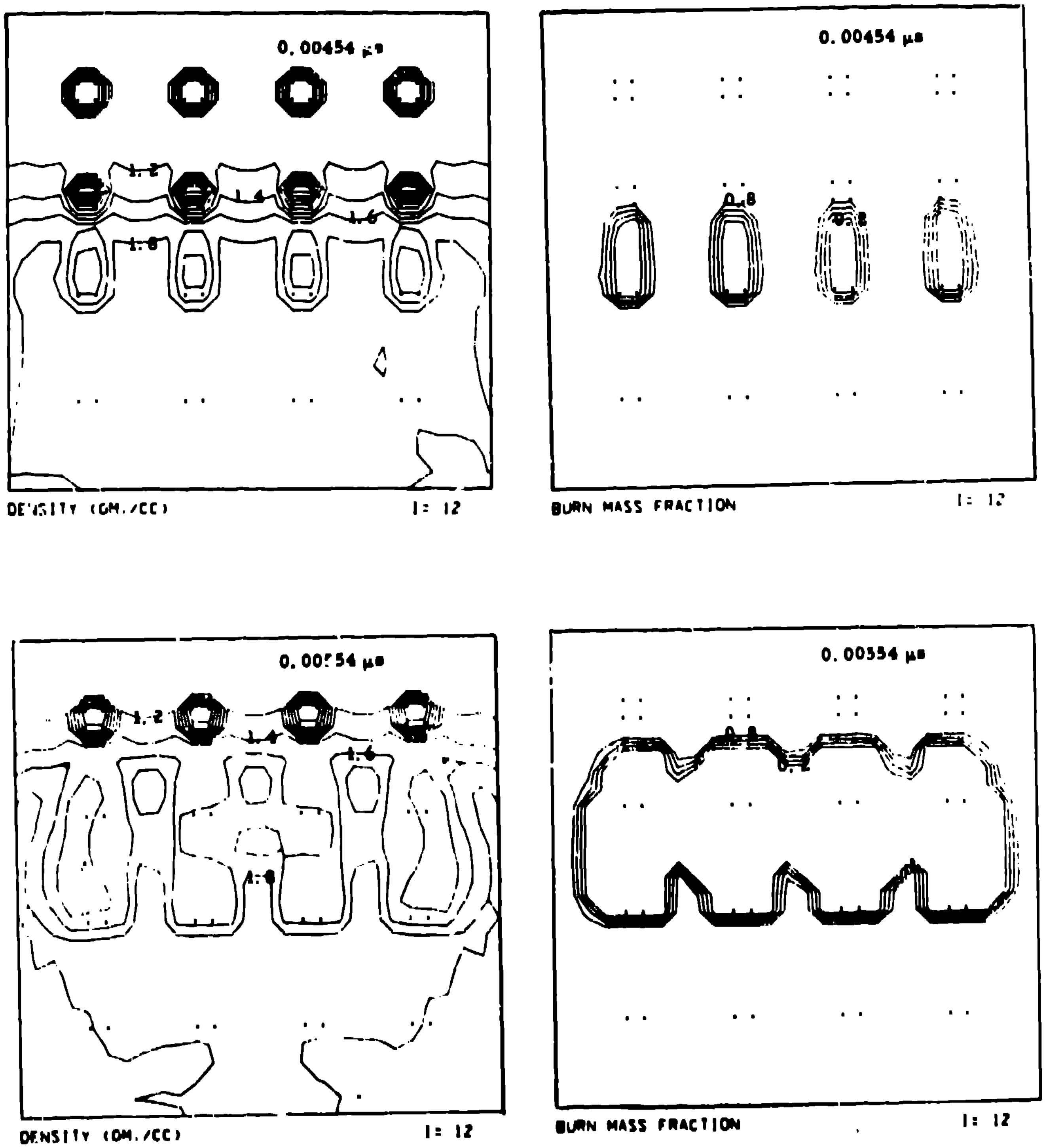
0.00454 μs
BURN MASS FRACTION
I: 12

Mader - Fig. 4



Mader - Fig. 5 p. 1



Mader - Fig. 5, p.2