Article

Oscillation transition in decay process of overdriven detonation

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Abstract

Numerical simulations of one-dimensional and two-dimensional detonations have been performed with two-step chemical reaction mechanisms for a stoichiometric hydrogen-air mixture at initial conditions of 42.7 kPa and 293 K. One-dimensional overdriven detonations are initiated by solutions of steady ZND detonations for degree of overdrive 1.1-2.0, and by shock compression with a piston for degree of overdrive 1.2. Shock pressure histories developing from steady detonations indicate high frequency oscillations for degree of overdrive 1.6-2.0 and low frequency oscillations for 1.1-1.5. In the piston initiation case, post-shock pressure is temporally led in a highly overdriven condition by penetration of an interior detonation and is gradually attenuated by incident rarefaction waves. In this decaying process of the overdriven detonation, both high frequency and low frequency oscillations are observed for the fixed degree of overdrive 1.2. The relation between the shock pressure and the oscillation characteristics such as period and pressure amplitude agrees with results of steady detonation initiations. An initiation process of a two-dimensional detonation from high pressure and temperature conditions is also numerically investigated. Oscillation characteristics on the center line of the cell in two-dimensional detonation indicate a similar transition to one-dimensional detonations in the decay process of initial overdriven conditions but do not depend on the shock pressure very much.

1. Introduction

Ballistic range experiments[1)-3)] in 1960s and 1970s revealed that the shock-induced combustion around the spherical projectile flying into the combustible gases has unsteady and periodic shock-reaction system. Those experiments show two oscillation modes[2) 3)] of shock wave-reaction front interactions: low amplitude and high frequency oscillations “regular regime” and high amplitude and low frequency ones “large-disturbance regime.” Toong and co-authors[2) 3)] first proposed periodic instability mechanisms based on experimental observation and one-dimensional wave interaction theory. Recently, computational fluid dynamics has been utilized to simulate the flow features of ballistic range experiments, and the mechanisms of the regular regime and the large-disturbance regime have been clarified by the CFD researches.[4)-8)] Matsuo and Fujii[6)] have indicated that not the projectile velocity but the intensity of the concentration of the heat release is the essential factor to determine the unsteadiness, and they newly proposed the wave interaction model for the large-disturbance regime.

One-dimensional piston supported flows have been also investigated employing numerous theoretical and computational analyses to understand the detonation phenomena.[9)-12)] These studies have close relevance to the unsteady structure of the ballistic range experiments. Fickett *et al*.[10)] found two oscillation modes in one-dimensional piston driven flows with a one-step irreversible reaction model. In the work of Sussman,[11)] the hydrogen-oxygen full chemistry is used for simulations, and the computed results show two modes by changing a degree of overdrive. Matsuo and Fujii[12)] indicated that the oscillation type did not depend on the intensity of the concentration of the heat release in contrast to the unsteadiness of the shock-induced combustion. Longitudinal oscillations of one-dimensional overdriven detonations are not restricted to gaseous detonations and reported on detonations in nitromethane and liquid TNT by Mader.[13)]

In almost all the previous studies of the one-dimensional piston supported detonation, solutions of steady detonations were used as initial conditions, and various waves reflected by the piston surface were neglected. The reflected waves, however, play important roles in the periodic mechanism in ballistic range experiments. The present study is carried out to clarify oscillation characteristics initiated by a steady solution, and by shock compression with a piston, taking into account of reflected waves at the piston surface. Under the same conditions as one-dimensional simulations, a two-dimensional simulation is performed and compared with one-dimensional longitudinal oscillations. Oscillation characteristics on the center line of cellular structures are examined for the discussion on the relation between one-dimensional and two-dimensional oscillations.

2. Computational Setup

One-dimensional and two-dimensional simulations are conducted using the Euler equations with the two-step chemistry model proposed by Korobeinikov.[14) 15)] Yee's non-MUSCL TVD upwind explicit scheme[16)] is used as a numerical scheme. The initial conditions are identical to Lehr's experiment[1)]: a stoichiometric gas mixture $2H_2+O_2+3.76N_2$ at initial pressure 42.7 kPa and initial temperature 293 K. Two-step reaction parameters in Table 1 are adopted for the mixture and under the parameter sets Chapman-Jouguet (C-J) detonation velocity D_{CJ} equals to 1938.3 m/s. Post-shock conditions and piston speeds are presented in Table 2, which are calculated from one-dimensional solutions of steady detonations for a given degree of overdrive f.

As for one-dimensional simulations, two types of initiation process are attempted: employing steady ZND solutions as initial conditions (SD case); overdriving quiescent combustible gases by a piston (PI case). A coordinate system moves at the same speed as a piston surface and 8001 points in SD case and 20001 points in PI case are provided in the whole computational domain. Firstly, a grid resolution study in SD case is performed with 10, 20, 40, and 80 grid points per induction length L_{ind} for the degree of overdrive $f = (D/D_{CJ})^2 = 2.0$, where D and D_{CJ} are overdriven and C-J detonation velocities. Then oscillation characteristics are investigated for degrees of overdrive between 1.1 and 2.0 at intervals of 0.1 in SD case and a fixed degree of overdrive 1.2 in PI case. The case of $f = 1.0$ in SD case is excluded from simulation conditions because the induction time and length are extremely increased and the shock wave-reaction front interaction is not observed in the computational domain. A detonation front of PI case is gradually attenuated by incident rarefaction waves and local characteristics in the decay process are examined and compared with stable characteristics of SD case.

A two-dimensional simulation is performed in a computational domain 300×7.5 L_{ind} (108×2.7 mm). The domain is discretized into 3001×51 grid points with grid resolution along x axis of 10 points per induction length L_{ind} (Table 1, $f = 1.0$) in a laboratory coordinate system: mesh size Δx = 36.0 μm; $\Delta y/\Delta x$ = 1.5. The benchmark result is compared against a result with a fine mesh of 4501×76 grid points (15 points / L_{ind}). The detonation is initiated by high pressure (3.0 MPa) and high temperature (3000 K) region which have 30×41 grid points (in fine mesh, 45×61) bounded on the left (x = 0.0 mm) and top (y = 2.7 mm) boundaries.

Table 1 Reaction parameter sets[14) 15)] for the stoichiometric mixture $2H_2+O_2+3.76N_2$ at initial pressure 42.7 kPa and initial temperature 293 K.

Q (exothermicity)	2.330×10^6 J kg^{-1}
R (gas constant)	397.6 J kg^{-1} K^{-1}
E_1/R (activation energy)	9850 K
E_2/R (activation energy)	2000 K
k_1 (rate constant)	3.000×108 m^3 kg^{-1} s^{-1}
k_2 (rate constant)	7.549×10^{-6} m^4 N^{-2} s^{-1}
γ (specific heat ratio)	1.4

Table 2 Post-shock conditions for a given degree of overdrive f (D, Detonation velocity; P_{ss}, Shock pressure; L_{ind}, Induction length; τ_{ind}, Induction time).

f	D, m s^{-1}	P_{ss},MPa	L_{ind}, μm	τ_{ind}, ns
1.0	1938*	1.14	360	915
1.1	2033	1.25	227	560
1.2	2123	1.37	154	368
1.3	2210	1.48	110	255
1.4	2293	1.60	81.9	186
1.5	2374	1.71	63.4	140
1.6	2452	1.83	50.5	109
1.7	2527	1.94	41.3	87.0
1.8	2601	2.06	34.5	71.1
1.9	2672	2.17	29.4	59.3
2.0	2741	2.29	25.4	50.2

*Chapman-Jouguet detonation velocity

3. Results and Discussion

3.1 Oscillation characteristics of detonations developed from steady detonation solutions (SD)

In order to reproduce accurate unsteady oscillations, it is necessary to determine the grid spacing required for adequate resolution of flow features. The grid resolution study is performed in SD case on successively decreased grid spacing of 10, 20, 40, and 80 grid points per L_{ind}. Especially 16001 grid points are provided for the grid resolution with 80 points per L_{ind}. For degree of overdrive f = 2.0, expected oscillation characteristics are low amplitude and high frequency oscillations; the high frequency mode. On the coarsest grid with 10 points per L_{ind}, the computed oscillation mode is not accurate high frequency oscillations, but on the three successively finer spacing of 20, 40,

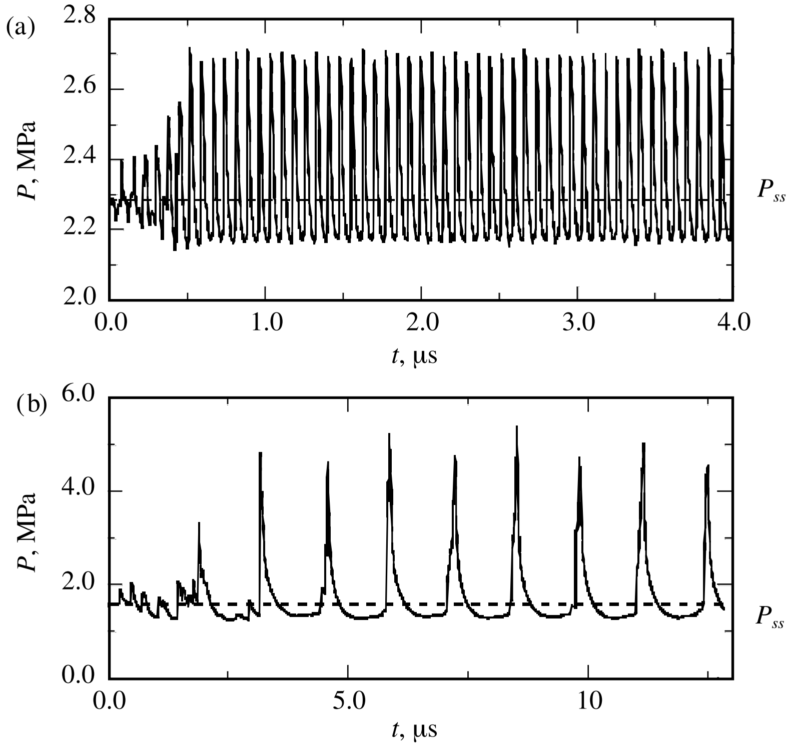

Fig. 1 Shock pressure histories in SD case, (a) f = 2.0, (b) f = 1.4.

and 80 grid points per L_{ind}, oscillation characteristics accord with the high frequency mode. On the grids with both 40 points and 80 points per L_{ind}, it is confirmed that those solutions are sufficiently converged into the same oscillations characteristics; the normalized oscillation period by the induction time τ / τ_{ind} = 1.47 and the normalized amplitude by the post-shock pressure ΔP / P_{ss} = 0.230. The following one-dimensional results are simulated with the grid with 40 points per L_{ind}.

Figures 1(a) and 1(b) show the histories of the shock pressure for f = 2.0 and 1.4, respectively. Figure 1(a) shows the typical oscillation characteristics of the high frequency mode. In the high frequency oscillations, amplitudes ΔP normalized by the shock pressure P_{ss} of steady solutions are about 0.25, and periods τ normalized by the induction time τ_{ind} are approximately 1.5 for f = 1.6-2.0. For f = 1.1-1.5, the oscillations have high amplitude and low frequency (low frequency mode) as shown in Fig. 1(b). The normalized amplitudes ΔP / P_{ss} are 1.0-4.0, and periods τ / τ_{ind} range from 7.0 to 25.0. These numerical results show that the oscillation mode depends on the degree of overdrive as well as the previous investigations.[6)-8)]

3.2 Oscillation transition of a detonation devel oped from piston initiation (PI)

Figure 2 is the x-t diagram of the density gradient in a piston surface stationary frame, and clearly shows the wave patterns in the whole computational domain for degree of overdrive f = 1.2. In Fig. 2, the shock is initiated by the piston at time 0.0 s, and the strong reaction front that is an interior detonation occurs at time 9.1 μs. The reaction front penetrates the shock front at time 11.3 μs, and simultaneously the strong rarefaction wave occurs and travels to the piston surface. After the penetration, oscillations of the shock front gradually appear, and periods of the oscillations become longer and longer. A series of compression waves and contact discontinuities, which are released from the shock front, can be also seen in Fig. 2. Between time 14.0 and 27.5 μs, two kinds of oscillation modes are observed. Figures 3(a) and 3(b) are the close-up view of Fig. 2 and exhibit the density contour distributions around the shock front. According to previous numerical

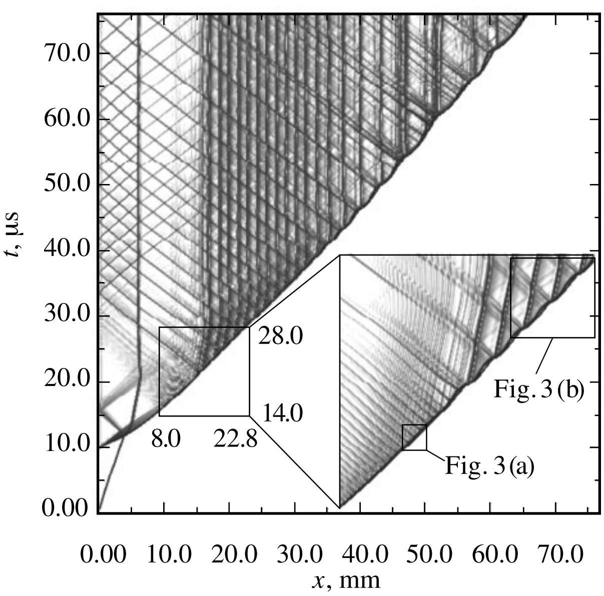

Fig. 2 x-t diagram of density gradient in PI case for f = 1.2.

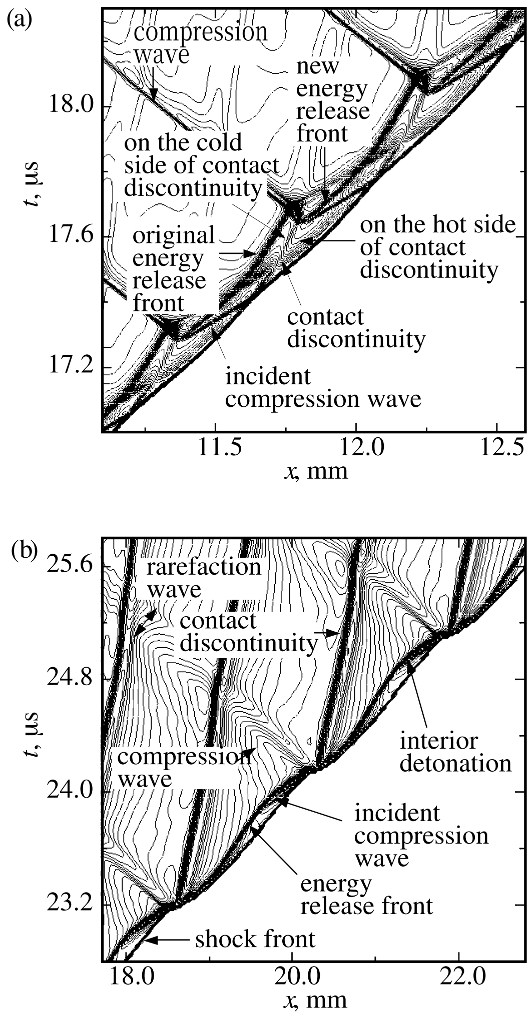

Fig. 3 Enlargement of Fig. 2, (a) high frequency mode, (b) low frequency mode.

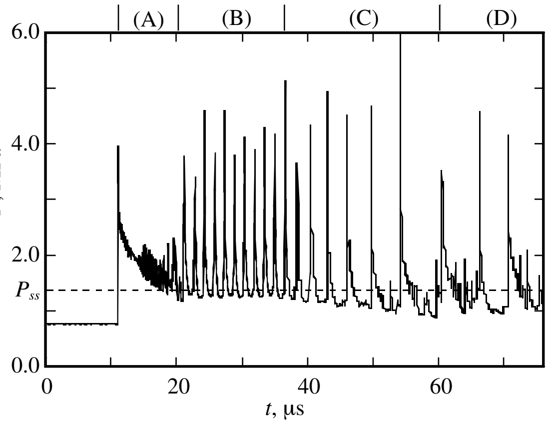

Fig. 4 Shock pressure history in PI case for $f = 1.2$.

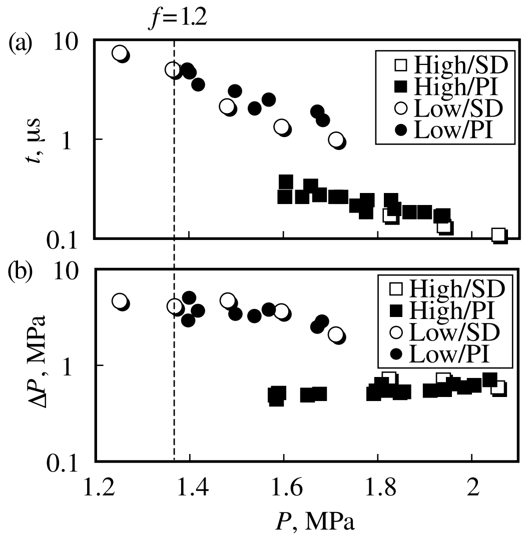

Fig. 5 Relation between shock pressure P and oscillation characteristics; (a) period τ and (b) amplitude ΔP.

results of unsteady combustions around a blunt body projectile,[4) 5)] Figs. 3(a) and 3(b) are classified into the interaction mechanisms of the high frequency mode and the low frequency mode, respectively. The transition from the high frequency mode to the low frequency mode occurs under the fixed degree of overdrive 1.2 while the unique oscillation mode is observed for a given degree of overdrive in SD case.

The history of the shock pressure is presented in Fig. 4 to discuss the reason of the mode-transition from the high frequency mode to the low frequency mode. First, the pressure level is constant and it is supported by the piston. Then, the shock pressure suddenly shows the peak due to the penetration of the reaction front. Since the rarefaction wave that propagates just behind the interior detonation attenuates the leading shock, in a domain (A) shock pressure gradually decreases and the flow feature indicate the high frequency mode as shown in Fig. 3(a). After the first incidence of the rarefaction wave in a domain (B), shock pressure becomes constant about 1.70 MPa, and the flow feature indicates the low frequency mode in Fig. 3(b). In a domain (C) average shock pressure is attenuated by the second rarefaction wave that is originated in the penetration of reaction waves and is reflected off the piston surface. Average pressure in a domain (D) becomes constant 1.39 MPa and the irregular oscillations occur, which is also observed in the previous numerical results of unsteady combustions around a cylindrical projectile.[17)] Average pressure and the flow feature of PI in the domain (D) agree well with the shock pressure of SD case (1.37 MPa, P_{ss}) for the degree of overdrive 1.2. Although the average pressure in SD is constant for each degree of overdrive, the local average pressure in PI case decreases as a function of time. This suggests that the mode-transition in PI is due to decreasing the local average pressure. Accordingly, the periods and the amplitudes of the oscillations are derived from the shock pressure history in Fig. 4 and are plotted in Fig 5(a) and 5(b) with those in SD case. The plots of SD case are computed values for degree of overdrive between 1.1 and 1.8, and are clearly divided into two oscillation modes around 1.75 MPa. The oscillation periods τ and amplitudes ΔP against the shock pressure in PI case are in well agreement with those in SD case, except for the transitional zone between 1.6 to 1.8 MPa. It is confirmed that longitudinal oscillation characteristics of the one-dimensional overdriven detonations have the strong dependence on the shock pressure.

3.3 Oscillation characteristics of a two-dimensional detonation

Figure 6 shows cellular structures of a detonation in the form of the gray scale of the frontal shock velocity in the x axis. The tone in a domain (i) is generally darker than those of the rest of domains (ii)-(iv). This implies that the detonation initiated by the high pressure and temperature region leads temporally overdriven state in the domain (i) during x = 0.0–32 mm. The tone becomes lighter as the detonation propagates, and thus the overdriven detonation is gradually attenuated. In the decaying process, cellular structures in the domain (ii) (x = 32–54 mm) have well-defined two triple points, and after the transition region (iii) (x = 54–74 mm) only one triple point propagates in the domain (iv). Although the initiation process of the two-dimensional detonation is different from the PI case in the one-dimensional overdriven detonation, the similar transition of oscillation characteristics appears in both detonations.

On the bottom boundary (y = 0.0 mm), shock pressure P can be derived from the equation for the pressure ratio across the normal shock in terms of the frontal Mach number along x axis. Degree of overdrive f and frontal Mach number along x axis are obtained from the frontal shock velocity in Fig. 6. Since shock pressure P is given as a linear function of degree of overdrive f, histories of P and f along x axis are drawn on the same profile with double axes in Fig. 7(a). In the history, the shock pressure P (solid line) oscillates from 0.36 MPa to 3.08 MPa, and the average pressure $P_{Ave.}$ (dotted line) gradually decreases to the post-shock pressure P_{ss} (= 1.14 MPa) of steady C-J detonations. Degree of overdrive f (solid line) along x axis varies from 0.4 to 2.7 and the average degree of overdrive $f_{Ave.}$ (dotted line) asymptoticaly decreases from 1.64 to almost 1.0. Since well-defined cellular structures appear in the domain (ii) (15-26 μs) and the domain (iv) (after 37 μs), oscillation characteristics are examined during those domains. In the domain (ii), P_{Ave}. equals to 1.30 MPa, and ΔP (= 2.00 MPa) is close to 2.05 MPa in SD case for f = 1.5. Average degree of overdrive f_{Ave}. equals to 1.14, and oscillation period τ equals to 2.84 μs. In the domain (iv), P_{Ave}. decreases to 1.17 MPa ($\fallingdotseq P_{ss}$) and ΔP decreases to 1.89 MPa. Average degree of overdrive $f_{Ave.}$ becomes 1.02 and oscillation period τ increases to 5.25 μs. Although ΔP in one-dimensional overdriven detonations increases with decreasing shock pressures, ΔP in the two-dimensional detonation does not. Oscillation characteristics in the two-dimensional detonation do not depend on the shock pressure very much.

Average propagation velocities of transverse waves along y axis are readily derived from the aspect ratio of the cell in Fig. 6. Aspect ratios in the domains (ii) and (iv) are 2.06 and 1.90, respectively and thus average velocities of transverse waves in those domains are 1006 and 1030 m s^{-1}. Hence the magnitudes of degree of overdrive on the triple point in the oblique direction are 1.41 and 1.30, taking into consideration both normal and parallel degree of overdrives to the propagation direction. For f = 1.41 and 1.30, oscillation periods τ are 1.41 μs and 2.13 μs, which are obtained from interpolations of SD case. Double of those oscillation periods become 2.82 μs and 4.26 μs and comparatively close to oscillation periods on the center line of the cell in the domains (ii) and (iv). The above features would imply that two-dimensional oscillation characteristics are relevant to the degree of overdrive of the triple point. Oscillation characteristics of the benchmark results (10 points/L_{ind}) are compared with the results with the finer mesh (15 points/L_{ind}). Histories of the shock pressure and the degree of overdrive along x axis (y = 0.0 mm) are drawn in Fig. 7(b). It is confirmed that oscillation characteristics with the fine mesh indicate similar mode transition to the benchmark results in the domains (i)-(iii) and well agree with the benchmark results in the domain (iv); τ= 5.16 μs and ΔP = 2.26 MPa. In the present study, the channel width is fixed to only one case 7.5 L_{ind}. It has been reported that the channel width plays important role to the transverse wave structures within the narrow channel where a few triple points appear.[18] Further parametric

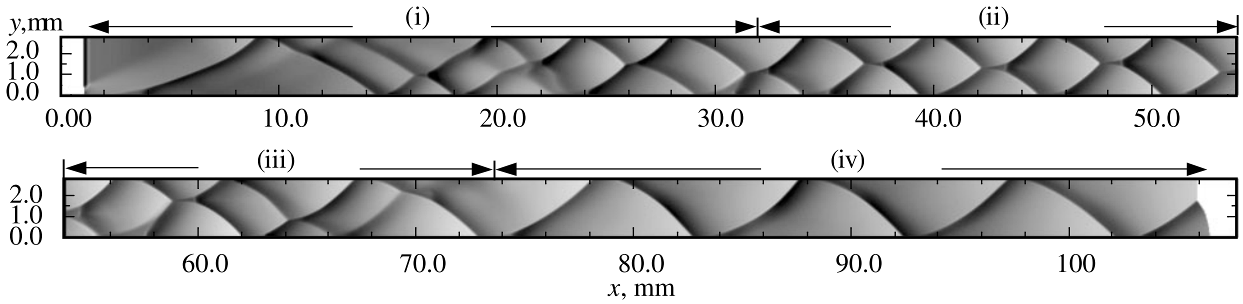

Fig. 6 Two-dimensional cellular structures in the form of gray scale distribution of the frontal velocity.
(Detonation propagates from the left boundary to the right boundary. The darker color indicates the faster velocity.)

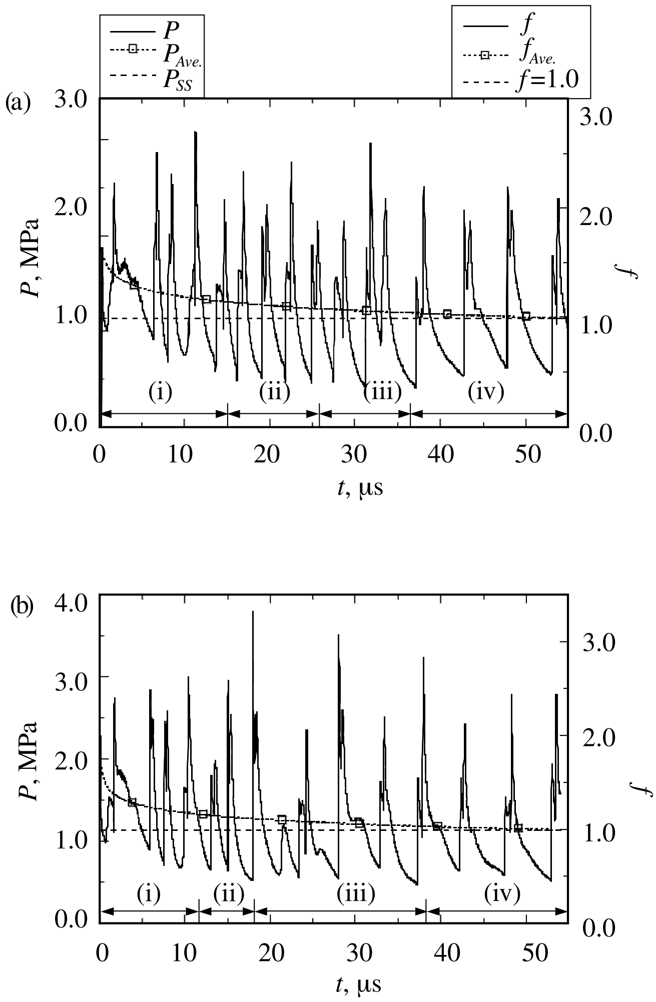

Fig. 7 Histories of shock pressure and degree of overdrive along x axis (y = 0.0 mm) (a) with the benchmark mesh (10 grid points/L_{ind}), (b) with the fine mesh (15 grid points/L_{ind}).

study on the initiation process of two-dimensional detonations would clarify the detail relation between two-dimensional oscillation characteristics and the degree of overdrive on the triple point.

4. Conclusions

One-dimensional overdriven detonations and a two-dimensional detonation were successfully simulated with two-step reaction mechanisms for stoichiometric hydrogen-air mixture at 42.7 kPa and 293 K. Two kinds of unsteady oscillations observed in unsteady combustions around blunt body projectile were also observed in one-dimensional overdriven detonations. The calculation started from steady solutions of propagating detonations indicated high frequency and low amplitude oscillations for degree of overdrive from 1.6 to 2.0, and low frequency and high amplitude oscillations for degree of overdrive from 1.1 to 1.5. The calculation started from overdriving quiescent combustible gases by a piston for the fixed degree of overdrive 1.2 exhibited two oscillation modes, depending on the local shock pressure. The relation between the local average pressure and the oscillation characteristics such as period and amplitude in the piston initiation case was in good agreement with those of the oscillations developed from steady detonations, except for the transitional pressure range. Although the initiation process of the two-dimensional detonation was different from the piston initiation case of the one-dimensional overdriven detonation, the similar transition of oscillation characteristics appeared in both detonations. Oscillation characteristics on the center line of the cell did not depend on the shock pressure very much, but suggested that they were relevant to the degree of overdrive on the triple point.

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