Temperature measurement and chemical reaction observation in combustion gas by X-ray Compton scattering

Recent automobile technologies require elucidation of complex combustion phenomena to achieve cleaner exhaust gas and less carbon dioxide emission. The combustion occurs owing to complex interactions involving heat, mass, and momentum transfer. The local flow temperature is a key factor for elucidating complex phenomena and must be accurately measured. Nonintrusive temperature measurements offer important advantages in the elucidation of combusting flows since they do not affect the flow characteristics and change the temperature distribution. Holographic temperature measurements have been suggested as a mean of accurately determining the refractive index in flames in order to infer the temperature distribution [1]. However, these measurements are sensitive to mechanical noise; hence, it is not easy to obtain accurate temperature data using a combustion instrument.

High-energy X-ray Compton scattering can be used for the nonintrusive measurement of the temperature distribution in the combustion gas of a flame with high accuracy and robustness because it does not have the drawbacks of an interferometric instrument. In this study, we developed a method of temperature measurement and chemical reaction observation for combustion flames using X-ray Compton scattering.

The experiment was performed at SPring-8 **BL08W** [2,3]. A cylindrical Bunsen burner (inner diameter, $d_{in} = 10$ mm) was used to provide a laminar mixture of propane (6 wt%, 450 ml/min) and air (94 wt%, 8 l/min). The burner provided a laminar propane/air jet at the outlet. The air and combustible gases were pure synthetic gases.

Figure 1(a) shows a side view of the self-sustaining flame. The bright flame front, at which CH* and OH* radicals emit light [4], has a cone shape. Figure 1(b) shows a cross-sectional map of the temperature distribution along the cylindrical axis of the flame shown in Fig. 1(a). The ambient temperature of 298 K is almost constant in the inner flame region, which is shown as the blue triangular region in Fig. 1(b). Figure 1(b) shows that the temperature increases suddenly at the bright flame front shown in Fig. 1(a), and reaches 1500 K just outside the flame. The temperature distribution shown in Fig. 1(b) was compared with those obtained using conventional thermocouples. The results indicate that temperature measurement using Compton scattering enables more precise measurement than that using thermocouples. This is because it is a noncontact method and there is no effect of thermal inflow from the thermocouple wire on the measurement.

In addition, analysis of the spectra of Compton-scattered X-rays enables chemical reaction measurement. Figure 2 shows differences in Compton profiles $\Delta J_{x\mathrm{mm}}(p)$ between $x = 0$ mm (where the gas is a mixture of air and the combustion gas at ambient temperature) and x mm (where the gas is undergoing the combustion reaction) at $y = 5$ mm. $\Delta J_{x\mathrm{mm}}(p)$ for $x = 4$ mm, just inside the combustion reaction zone, is almost zero within the range of experimental error.

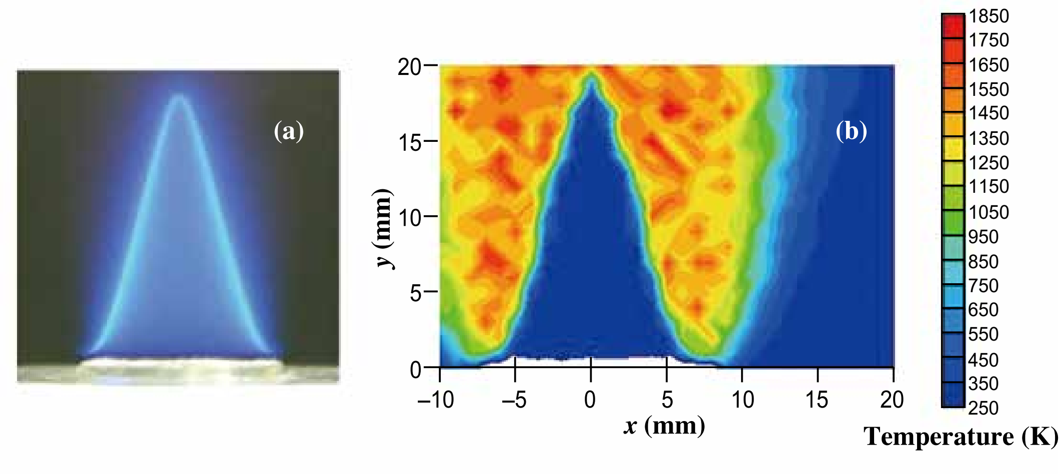

Fig. 1. **(a)** Photograph of self-sustaining flame. **(b)** Cross-sectional map along the cylindrical axis of the flame shown in (a). The flame center is at $x = 0$ mm.

This shows that the chemical reaction does not take place. This is consistent with the fact that the ambient temperature of 298 K remains almost constant just inside the combustion reaction zone, as shown in Fig. 1(b). It should be noted that $\Delta J_{xmm}(p)$ in the combustion reaction zone ($x = 4.5$ mm) is almost zero within the range of experimental error, although bright luminescence in the combustion reaction zone is observed, as shown in Fig. 1(a) and the temperature is 800 K, as shown in Fig. 1(b). This suggests that the main type of chemical bonding remains, but a combustion reaction, such as radical luminescence, starts at the combustion reaction zone. $\Delta J_{xmm}(p)$ just outside the combustion reaction zone ($x = 5$ mm) deviates from zero. This indicates that the main type of chemical bonding, or molecular species, has changed drastically. This means that the combustion reactions are complete just outside the combustion reaction zone and that a 1500 K high temperature region without luminescence extends into the outer region of the combustion reaction zone as a result of the flame gas flow.

The calculated $\Delta J_{xmm}(p)$ for $x = 5$ mm assuming the following ideal chemical reaction [1] and using CRYSTAL09 codes [5] is also shown in Fig. 2(c) by the solid line.

$$C_3H_8 + 7.8(O_2 + 3.76N_2) \rightarrow 3CO_2 + 4H_2O + 29.3N_2 + 2.8O_2$$

Although the dip structure for $|p| < 0.5$ a.u. seems to be reproduced by the calculation, positive values with $|p| < 1$ a.u. and negative values with $|p| > 1$ a.u. are not reproduced. Through the comparison of further Compton profiles calculated using CRYSTAL09 codes [5] for air (O_2+3.76N_2), CO_2, H_2O, and C_3H_8, and the Hartree-Fock calculation for atomic H [6], the deviation from the ideal chemical reaction can be explained by the presence of many atomic H with OH radical species [4].

This method can be used for noncontact measurement of the temperature distribution and chemical reactions in internal combustion engines because high-energy X-rays with high permeability are used in this analytical method. This measurement method is expected to help advance the development of innovative engine technology with improved efficiency.

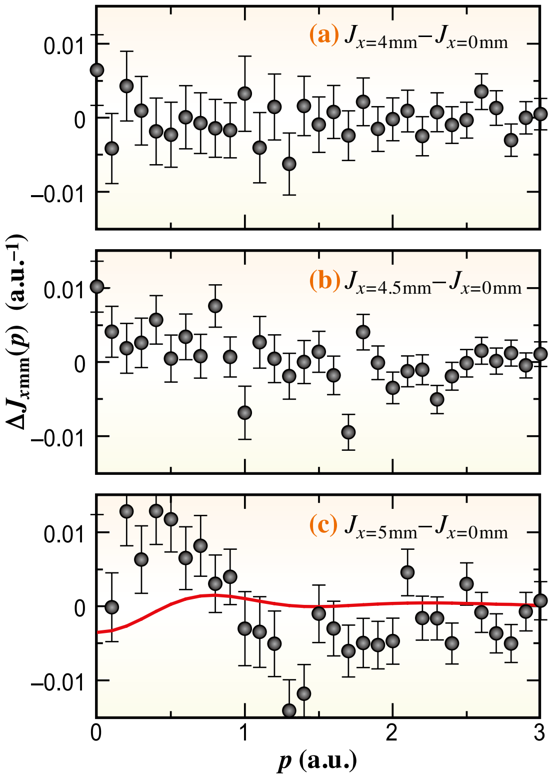

Fig. 2. Difference Compton profiles, $\Delta J_{xmm}(p)$, between a position at the center of the flame, $x = 0$ mm and **(a)** $x = 4$ mm (just inside the combustion reaction zone), **(b)** $x = 4.5$ mm (at the edge of the combustion reaction zone), and **(c)** $x = 5$ mm (just outside the combustion reaction zone) shown in Fig. 1(b). Here, $y = 5$ mm. The difference in the Compton profile calculated using CRYSTAL09 codes assuming the ideal chemical combustion reaction is shown by the solid line. p is the momentum.

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