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Physical and mathematical modeling of ignition, combustion and detonation of silane-hydrogen-air mixtures

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ABSTRACT

Studies of ignition limits, combustion and detonation of silane are now actual due to fire safety of industrial plants using silane. In particular, the silane is widely used in semiconductor industry as a source of silicon, which is obtained by combustion of silane. In this paper, the development of physical and mathematical model of ignition, combustion and detonation of the mixture of silane, hydrogen, oxygen and an inert gas (nitrogen, argon) is proposed, based on detailed kinetics. The comparison with experimental data on the ignition delay time of silane, hydrogen, oxygen and nitrogen mixture versus temperature behind the reflected shock wave through the three criteria of ignition of the mixture showed that the model with detailed chemical kinetics satisfactorily describe the experimental data. Furthermore, the ignition limits (upper and lower) of the mixture of silane - oxygen and silane - air at pressures from 0.05 to 1.1 atm and temperatures between 350 and 640 K on the basis of detailed chemical kinetics model were found. The effect of the silane - air mixture composition on the ignition limits was found. It was shown that the increasing of silane amount in mixture change the critical temperature of ignition non-monotonically.

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1. Introduction

Silane is one of the most widely used silicon source gases in the semiconductor industry and has unpredictable ignition behavior (Chen et al., 2006; Tamanini et al., 1998). Silane-air mixture is able to self-ignite even at room temperature. The probability of an explosion depends on a wide range of parameters. The set and the value of the parameters have not been systematically investigated. For example, silane-air explosion probability depends on the temperature, velocity of the mixture, ambient humidity, etc. Thus, silane-air mixtures are the source of permanent explosion hazard. This emphasizes the importance of investigation of ignition, explosion and detonation parameters of silane-air mixtures to solve the corresponding problems of explosion and fire safety. Moreover, recently, silane considered as the initiator of hydrogen ignition which used as fuel in the supersonic engines.

Silane ignition and combustion have been studied since the 1930s (Shantorovich, 1935). The studies of ignition and combustion of silane included self-ignition (Hartman et al., 1987; Kondo et al.,

2000), laminar flame propagation (Tokuhashi et al., 1990) and ignition behind the reflected shock waves (McLain et al., 1983). From the literature it is known a certain amount of works on modeling of ignition and combustion of silane. Jachimowski and McLain (1983) developed kinetic model based on analogies with methane oxidation. It was used to predict the dependence of ignition delay time in mixtures of silane/hydrogen/oxygen/nitrogen on the temperature. Later the same calculations were made by Chinitz (1985) and Golovitchev and Bruno (1998) on the basis of more complex detailed chemical kinetics models (90 and 134 forward and reverse reactions, respectively). In the papers the effect of the silane addition to a mixture of hydrogen/oxygen/nitrogen on the ignition delay times at temperatures ranging from 800 to 1250 K and pressures ranging from 0.5 to 1.35 atm was studied. For these purposes series of calculations of ignition delay times of hydrogen-silane mixtures with oxidizer in the range of mixture compounds from pure hydrogen/oxygen/nitrogen mixture to pure silane/oxygen/nitrogen mixture were performed. Calculations have shown that the addition of small amount of silane (to 20%) in mixture of hydrogen/oxygen/nitrogen greatly decreases the ignition delay times of mixtures. Further increase in the amount of silane in the mixture (from 20% to 100%) only slightly changes the ignition delay times.

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Later the model provided by Jachimowski and McLain (1983) was used by Tokuhashi et al. (1990) for calculation of burning velocities of silane laminar flame. Britten et al. (1990) developed a kinetic model, which takes into account a 140 elementary chemical reactions. This model make it possible to explain experimentally observed ignition delay times at low mixture pressures (20–100 kPa) and temperatures (373–413 K). Kondo et al. (2000) made modification of Britten et al. (1990) scheme and studied an ignition of silane at room temperatures. It was shown that existence of self-ignition of silane at room temperatures depends on ratio of amount of fuel to oxidizer. Miller et al. (2004) proposed more complex chemical kinetic model, which takes into account 201 elementary reactions for 69 components. Using this model, he tried to describe experimentally observed times needed to rich maximum of radical OH at ignition of mixtures of hydrogen-oxygen, silane-oxygen and silane-hydrogen-oxygen. But a good agreement with the experimental data was obtained only for hydrogen-oxygen mixture, for all other mixtures a big differences between calculated and experimental data were obtained.

In this paper, the construction of physical and mathematical models of ignition and combustion of the mixture of silane/hydrogen/air in the reflected shock waves is proposed, based on detailed chemical kinetics. Ignition delay times and detonation velocity in mixtures of silane/hydrogen/air are calculated. The ignition limits (upper and lower) of the mixture of silane - oxygen and silane - air at pressures from 0.05 to 1.1 atm and temperatures between 350 and 640 K on the basis of detailed chemical kinetics model were found. The effect of the silane - air mixture composition on the ignition limits was determined too. These results can be used in solutions of problems of explosion- and fire safety.

2. Physical and mathematical model of ignition and combustion of silane

Let us consider a shock tube filled with a mixture of silane, hydrogen, oxygen and nitrogen/argon. Let a shock wave (SW) propagates over the mixture. Under certain conditions on the SW Mach number, the parameters of the mixture can exceed the critical conditions and ignition process will occur.

In 1D approach the dynamics of the mixture is described by equations of nonequilibrium gas dynamics:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} &= 0, \\ \frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + p)}{\partial x} &= 0, \\ \frac{\partial(\rho E)}{\partial t} + \frac{\partial[(\rho E + p)u]}{\partial x} &= 0, \end{aligned} \quad (1)$$

where $E = e + \frac{u^2}{2}$ – total energy of gas mixture, ρ , u , p , e – density, velocity, pressure and internal energy of gas mixture, respectively. The internal energy of reacting gas mixture is determined by the relation

$$e = c_v(T)T + \sum_{\alpha=1}^N \xi_{\alpha} h_{0\alpha} - c_p(T)T_{00}$$

where $c_p(T)$, $c_v(T)$ – specific heats of the mixture at constant pressure and volume respectively, ξ_{α} – relative mass fraction of the species α , $c_v(T) = \sum_{\alpha=1}^N c_{v\alpha}(T)\xi_{\alpha}$, $h_{0\alpha}$ – enthalpy of formation of species α , N – number of mixture components, $T_{00} = 298.15$ K. Data of the dependencies of specific heats on mixture temperature were taken from NIST Chemistry WebBook and from work of Rutz and

Bockhorn (2007). Data of the enthalpy of formation were taken from NIST Chemistry WebBook. System (1), supplemented with the equation of state

$$p = \rho TR \sum_{\alpha=1}^N \frac{\xi_{\alpha}}{M_{\alpha}}, \quad (2)$$

and the equations of detailed chemical kinetics

$$\begin{aligned} \frac{d\xi_{\alpha}}{dt} = \frac{1}{\rho} M_{\alpha} \sum_{r=1}^l \rho^{m_r} (v'_{\alpha r} - v_{\alpha r}) & \left[k_{fr} \prod_{\beta=1}^N \left(\frac{\xi_{\beta}}{M_{\beta}} \right)^{v_{\beta r}} \right. \\ & \left. - k_{br} \prod_{\beta=1}^N \left(\frac{\xi_{\beta}}{M_{\beta}} \right)^{v'_{\beta r}} \right]. \end{aligned} \quad (3)$$

To describe the kinetics of ignition and combustion of silane-air mixture we use the slightly modified detailed chemical kinetics provided by Britten et al. (1990), which contains 140 forward and reverse reactions of 25 components (H_2 , O_2 , H_2O , OH , O , H , HO_2 , H_2O_2 , SiH_4 , SiH_3 , SiH_2 , $HSiO$, SiH_2O , SiH_3O , SiH_3O_2 , $xSiH_3O_2$, SiH_3OH , SiH_3O_2H , SiH_2OH , $HSiOOH$, $SiOOH$, SiO , SiO_2 , N_2 , Ar). The reaction rates of forward and reverse reactions presented in work of Britten et al. (1990), the new data on activation energy of some reactions ($SiH_3O_2 \rightleftharpoons SiH_2O + OH$, $HSiOOH + O_2 \rightleftharpoons SiOOH + HO_2$, $HSiOOH \rightleftharpoons SiOOH + H$) in the model we take from work by Kondo et al. (2000). It should be noted that in the model of Britten et al. (1990) the component SiO_2 is formed in the gas-phase reactions but with an enthalpy of formation taken for a solid phase. However, in the structure of detonation wave (DW), where relatively high temperatures (2000–3000 K), SiO_2 is in a gaseous phase. Therefore, we consider the enthalpy of formation of the component taken for a gas phase.

3. Results and discussion

3.1. Ignition delay times of silane. Verification of kinetic scheme

Let's consider the problem of ignition of the mixture behind the reflected SW. It is known that the flow behind the reflected SW is motionless, so the system (1) converted to the equation describing the change in temperature of the gas mixture:

$$\frac{dT}{dt} = -\frac{1}{c_V(T)} \sum_{\alpha=1}^N (c_{V,\alpha}(T)T + h_{0\alpha} - c_p(T)T_{00}) \frac{d\xi_{\alpha}}{dt}. \quad (4)$$

Thus, the ignition of the mixture behind the reflected SW is described by equations (2)–(4). Initial data at $t = 0$: $u = 0$, $p = p_r$, $T = T_r$, $\xi_{\alpha} = \xi_{\alpha,0}$.

There are several criteria to determine the ignition delay times. Earlier, by Fedorov et al. (2012) it was shown that different ignition criteria give very close results to each other for hydrogen/oxygen diluted by nitrogen/argon mixtures. Consider the data obtained by using some of them for silane/hydrogen/oxygen mixtures.

Criterion 1. Here, criterion for determining the ignition delay time in the calculations was the achievement of maximum growth of temperature of the mixture in time – $\max \left(\frac{dT}{dt} \right)$. Fig. 1 shows the

dependence of the ignition delay time of silane-hydrogen-oxygen-nitrogen mixtures on temperature behind the reflected SW, calculated using the model and obtained in the experiments of McLain et al. (1983). The experiments were carried out for different compounds of mixtures and parameters behind the reflected SW. Mixture 1: $\xi_{SiH_4} = 2.45 \cdot 10^{-2}$, $\xi_{H_2} = 6.12 \cdot 10^{-3}$, $\xi_{O_2} = 4.9 \cdot 10^{-2}$,

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