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Dissolution kinetics of carbon in aluminum droplet combustion: Implications for aluminized solid propellants

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Abstract

An analytical model describing the kinetics of carbon dissolution in burning aluminum droplets has been developed in order to simulate its effects under solid rocket motor conditions. A carbon dissolution rate (k) was introduced in different droplet regression laws and depending on the heterogeneous kinetics between the Al surface and the surrounding gases. The model was validated using previous experiments performed by the authors on millimeter-sized Al droplets burning in several CO_2-containing atmospheres at atmospheric pressure ($P = 1$ atm). It has been shown that the carbon dissolution is affected by the presence of hydrogen due to competition between CO and H_2 chemisorption. The model was then applied to aluminized propellants (AP/HTPB) at high pressures ($P = 60$ atm) and high temperatures ($T = 3000$ and 3500 K), as well as at various burning rates and adsorption conditions. Though the accuracy of the extrapolation results needs further improvement, it has been shown that the carbon dissolution process should not be neglected in order to achieve global understanding of the combustion of Al particles, particularly agglomerates.

Keywords: Aluminum; Combustion; Carbon; Dissolution; Kinetics; Solid propellant

1. Introduction

The dissolution of carbon in aluminum droplets burning in CO_2-containing atmospheres was demonstrated in recent works [1–3]. This phenomenon is important because the amount of carbon dissolved in liquid aluminum is significant (≈20% mol C at $P = 1$ atm), and it has to be taken into account to understand combustion processes, particularly in aluminized solid propellants (P_{CO_x} up to 20 atm during the decomposition of AP/HTPB). Two main effects of carbon dissolution on Al burning are identified: First, an increase of the carbon concentration in the droplet decreases aluminum vaporization ($P_{Al}(x_C = 0.2)/P_{Al}(x_C = 0) \approx 0.75$ at $T = 2600$ K, [4,5]) and burning rates. Second, when the carbon concentration reaches its saturation limit, the excess carbon resulting from continuous droplet regression is ejected at the surface and forms a growing solid coating, which also prevents Al vaporization and gas-phase burning [2] (Fig. 1: Frames 1–7). A new combustion regime may therefore occur when the carbon coating interacts with the oxide cap, producing an aluminum oxycarbide phase (Fig. 1: Frames 8–10). In hot ambi-

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Nomenclature

a_i	dissolution parameter
b	probability of CO adsorption/C dissolution in Al
b_0	adsorption probability
C	carbon concentration, mol/mm^3
d	droplet diameter, mm
$\mathcal{D}_{\text{Al–C}}$	Al–C diffusion coefficient, mm^2/s
e_{H_2}	coefficient of H_2 poisoning
E_a	activation energy, eV
k	carbon dissolution rate, mm/s
k_P	carbon dissolution rate, mm/s/atm CO
k	Boltzmann constant, 1.381×10^{-23} J/K
n	exponent of the burning d^n law
N	dissolved carbon mole number, mol
P	pressure, atm
S	droplet surface, mm^2
t	time, s
T	temperature, K
V	droplet volume, mm^3
Z	quantity of CO chemisorbed on Al, $\text{molecules}/\text{mm}^2/\text{s}$
β	burning rate, mm^n/s
ρ	density, mg/mm^3
Φ	carbon flux, $\text{mol}/\text{mm}^2/\text{s}$

Subscripts and superscripts

°	without H_2
0	initial
Al	aluminum
b	burning
C	carbon
CO	carbon monoxide
CO_2	carbon dioxide
CO_x	CO and CO_2
d	droplet
H_2	dihydrogen
s	surface
sat	saturation
T	total

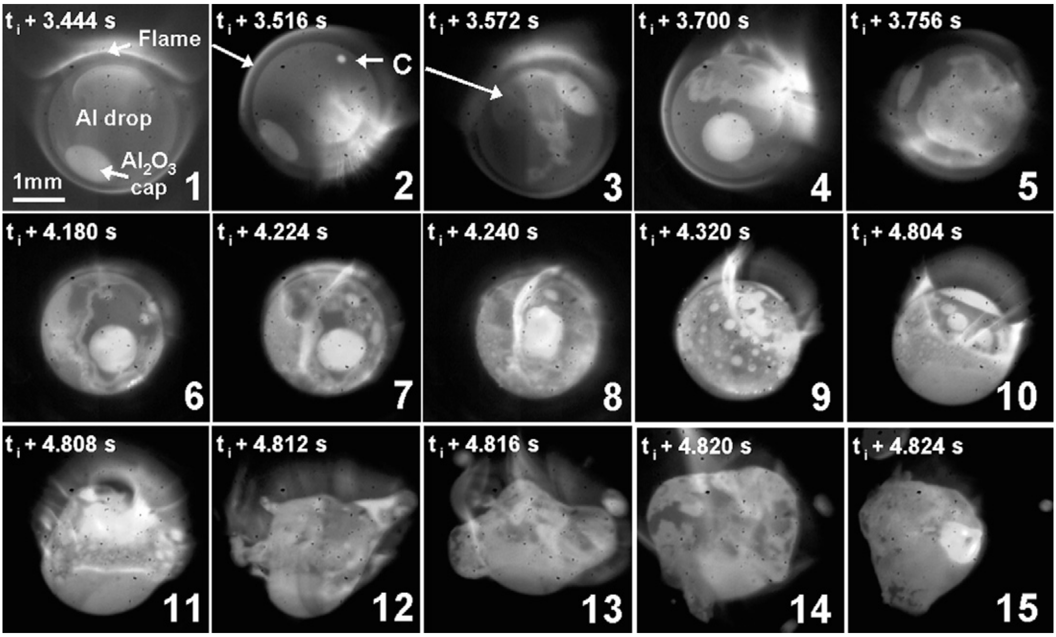

Fig. 1. Experimental pictures showing the carbon ejection process and its interaction with the oxide cap at the surface of an aluminum droplet burning in 100% CO_2.

ent gases, this phase can be melted, which promotes direct surface reactions. The droplet is then gradually oxidized, and dissolved carbon is finally released as CO from the residue, which may also be a source of fragmentation [3] (Fig. 1: Frames 11–15). In fact, the carbon ejection process initiates a change in the combustion regime (gas-phase to surface reactions), but it closely depends on the preliminary dissolution conditions occurring during the first burning stage.

In the present paper, a simplified analytical model is proposed in order to describe the kinetics of carbon dissolution during the combustion of aluminum