Simulation of catalytic properties of thermal barrier coatings for space vehicles in dissociated air

V.L.Kovalev, A.A.Krupnov

Lomonosov Moscow State University, Department of Mechanics and Mathematics, Institute of Mechanics

E-mail: valerykovalev@yandex.ru

Heterogeneous processes play a key role in controlling the heat flux to the surface of reusable space vehicles during their entry into the atmosphere. Elucidation of the mechanisms of these processes and determination of their basic kinetic characteristics are important for developing effective thermal protection systems.

The relevance of studies of the properties of thermal barrier coatings has been enhanced by the advent of new materials for promising reusable hypersonic aircraft, which need effective thermal protection at surface temperatures of ~2000 K. In addition, all the more challenging become the issues of reducing the heat load on the surface of spacecraft and probes designed to descend into the Martian atmosphere and then to return to Earth.

In this paper elementary stage rate coefficients of a complete set of a heterogeneous catalytic recombination in dissociated air on surfaces of thermal-protective ceramic tile coverings β-cristobalite and α-Al2O3 are defined by means of quantum mechanics calculations within the limits of cluster models . The processes of a shock (IR) and associative recombination (LH) of adatom of oxygen and nitrogen were considered.

The obtained values of the rate constants were used to calculate the values of the heterogeneous recombination probability on surface covers, and recombination heat flows for a diffusion layer near the surface under study at surface temperatures of 200–2000 K and pressures of 1000–7000 Pa.

Analysis of the results showed that the contributions from the two model mechanism cannot be rigorously separated in the entire temperature range, except for low temperatures (up to 800 K), where the ER mechanism dominates and high temperatures above 1000 K), where the LH mechanism provides up to 70% of the recombination probability.

The approaches grounded on usage of methods of quantum mechanics, allow to fathom better the gear of heterogeneous catalytic processes and to define rate coefficients of the elementary processes without engaging of experimental data.