Applied Surface Science 256 (2010) 6096–6106

Contents lists available at ScienceDirect

Applied Surface Science

journal homepage: www.elsevier.com/locate/apsusc

Numerical investigation on atomic oxygen undercutting of the protective polymer film using Monte Carlo approach

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ARTICLE INFO

Article history:
Received 7 March 2010
Received in revised form 24 March 2010
Accepted 24 March 2010
Available online 31 March 2010

Keywords:
Polymer film
Atomic oxygen undercutting
Monte Carlo
Numerical simulation

ABSTRACT

Atomic oxygen undercutting effect of the protective polymer film in low earth orbit space environment is a potential threat to vulnerable long duration exposure facility. A Monte Carlo computational model is developed to simulate the interactions between atomic oxygen undercutting course with polyimide film. Physical process of the atomic oxygen undercutting, the definition of parameters, the affected by atomic oxygen fluence, orbit angle, protection coating thickness and thermal assimilation and the additive anti-undercutting components as well as a new three-dimensional reaction probability are discussed in detail. Simulated results are in good agreement with flight experimental data. With the increment of the atomic oxygen fluence, all the undercutting profiles, the depth and the width increased. Maximum undercutting depth is always larger than maximum undercutting width and the larger thermal assimilation coefficient causes the smaller undercutting damage. Using three-dimensional reaction probability, maximum depth decreased by approximately 20% than that of 28.5° orbit angle.

1. Introduction

Atomic oxygen is the most abundant elements in the low earth orbit space environment. The sky lab mission and early shuttle flight data indicates that it is readily produce damaging erosion for exposed surfaces, especially for polymer materials [1–13]. Atomic oxygen undercutting is mainly originated from the attacking atoms, which have characteristics with the relative velocity of 8 km/s and the kinetic energy of 5 eV. The magnitude of energy is sufficient to break covalent chemical bonds, particularly in the case of hydrocarbon polymer film. For example, Kapton membrane had not only been damaged in larger mass loss but also in undercutting profiles. Its erosion can be augmented by several factors: solar ultraviolet irradiation, proton and electronic irradiation, thermal cycling and contamination of low earth orbit. The main consequences of atomic oxygen erosion are the degradation of thermal, mechanic and the optical properties characteristics for exposed materials [14–18]. These damages can lead to the failure of flight mission. Hence, they must be taken into accounted in the design stage. The most polymers that concerns about long term durability have been made efforts to develop for resisting to atomic attack, or atomic oxygen durable protective coatings which would prevent the underlying material from being attacked.

Efforts to evaluate the effectiveness of atomic oxygen protective coatings on polymers have been carried out in both ground test and space flight test in last decades. When atomic oxygen enters from the defect site (i.e. pin windows and cracks) in protective coatings on polymer, undercutting may be occurred by means of the oxidation actions, where its size maybe much greater than the initial size of the defects to some extent [19–22]. Because atomic oxygen reaction probability is primary dependent on its impact energy, the difference between the ground test impact energy and true low earth orbit space environment impact energy must be taken into account for performing the reliability validation in accordance with the ground test [23]. To a great extent, energy compensation method has been used to define the "effective atomic oxygen fluence" when measuring effects of atomic oxygen erosion. The effective atomic oxygen fluence is the number of impinging atoms per area that would be required in true low earth orbit space environment to produce the equivalent erosion effects, which can be observed in an arbitrary energy ground test system. Ground test systems should produce the equivalent atomic oxygen energies by providing many more actual atoms to simulate true erosion in low earth environment due to the limitation of the test conditions (i.e. expensive cost of equipment, expenditure of test and a longer period of test operation). Therefore,

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doi:10.1016/j.apsusc.2010.03.126

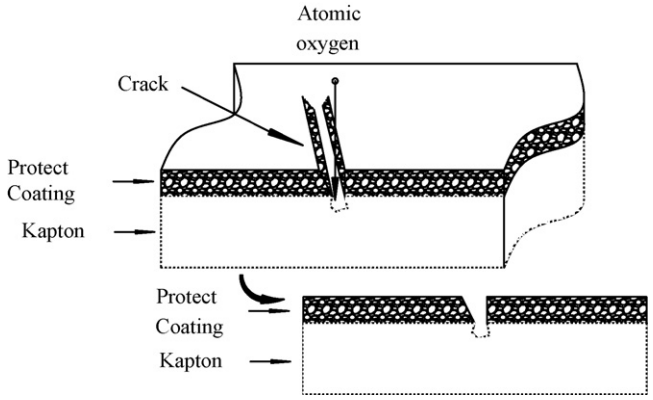

Fig. 1. Undercutting defect sites.

a reasonable physical and mathematical model as well as proper numerical simulation technique is of great importance for predicting and providing a large quantity accurate data for practical spacecraft design.

Atomic oxygen undercutting can be assumed to be the sum of the single atomic oxygen undercutting in terms of the statistical law. Monte Carlo model describing the interaction between atomic oxygen undercutting with polyimide Kapton film of spacecraft surfaces in low earth orbit has been widely used [24,25]. The aim of simulation is to accurately predict the undercutting patterns in both space and ground test in atomic oxygen environments and to provide a large amount of reference data for effective protection. In this study, investigation using a Monte Carlo model is performed to simulate atomic oxygen undercutting profiles under different orbit and space environment factors and the binary chained list optimization technique as well as the averaged error analysis of Monte Carlo are presented. Compared with the conventional two-dimensional reaction probability model, a new three-dimensional reaction probability model is established for discussing the undercutting differences.

2. Monte Carlo model of atomic oxygen undercutting

2.1. Physical process

Physical process of atomic oxygen undercutting is considered as a particle transport course. A cross-section of a portion of polymer is exposed to atomic oxygen environment and defect site in protective coating is attacked by simulated atomic oxygen. Because this model based on two-dimensional space position, every defect is considered crack or a scratch type shape and erosion occurred at microscope defects in protecting coating (see Fig. 1). Polymer is described by orthogonal array cells, where each of cells represents a group of polymer atoms which can potentially be oxidized. When model atomic oxygen atoms come into the defect site and the underlying polymer would be impinged, three possible events can be occurred due to impacting on a representative polymer model cell. They are as follows: (1) Cells are removed due to undercutting. (2) Un-reaction atoms are scattered. (3) Atoms are thermally assimilated. Probability of atomic oxygen reacting with the polymer cell is dependent upon the impact energy and the local attacking angle. Their reflection ways are in accordance with the cosine laws $\cos(\theta)^{1/2}$, where θ is the angle of impact relative to the normal of the slope averaged cell surfaces (see Fig. 3).

Un-reacted atomic oxygen will scatter from polymer surface according to the specular reflection or the diffuse reflection. Scattered un-reacted atomic oxygen atoms are free to potentially react at other locations within the undercut cavities or to escape from initial defect entrance. Since heat transfer between atomic oxygen and polymer occurs, thermally assimilated atomic oxygen will lose their kinetic energy and keep the same energy level for those thermal atoms.

Table 1
Parameters of undercutting simulation.

Initial impact-reaction probability during flight	0.1380
Initial impact-reaction probability in low energy stage of ground-based test simulator	0.0392
Thermal assimilation probability	0.0031
Reaction probability is direct proportion to the square root of cosine angle between incidence direction and normal direction of surface	$P=\cos(\theta)$
Reaction probability is direct proportion to the 0.68 power of AO energy	$P=E^{0.68}$
Ratio of AO thermal assimilation	0.5–1.0
Temperature of AO thermal assimilation	300
Temperature of space environment	1227 K

2.2. Determination of key parameters

Interaction parameters must be quantified for ensuring simulated results in agreement with experimental undercutting protected polyimide Kapton samples returned from the long duration exposure facility (LDEF). Initial reaction probability is mainly depends on the true atom energy and the activation energy. For ground test of atomic oxygen exposures, the initial impact energy is considered as the representation of the ground laboratory facility. Because each of model Monte Carlo atoms represents many true atoms and every Monte Carlo cell represents a measurable cross-sectional square of polymer, one must calibrate the Monte Carlo simulated exposure to draw meaningful conclusions from measured undercutting data. The assumption conditions are provided for obtaining accurately the key simulation parameters. They are defined by: (1) Atomic oxygen erosion is isotropy in everywhere of cells. (2) Thermal motion of atoms is taken into account and the mean free path of atoms is too lager to recombine the oxygen molecular. (3) Protection coating is not taken part in the oxidation reaction.

The key problem of Monte Carlo simulation is to determine the number of model atom for simulating erosion of unprotected materials in larger defects. The reason is that their space test data are reliability, such as the reaction coefficient of unprotected materials $\lambda = 3.0 \times 10^{-24}$ cm^3/atoms [21]. Numerical simulation results can be calibrated by these data. Assumptions course are as follows: The width of larger defect is $W_d = 50$ μm, length is L_d. W_d is grided by 500 unit cell and each unit cell represents 0.1 μm (see Fig. 2). The number of cell C is used for presenting L_d($C = L_d/L$). A model atom standing for the number of true atomic oxygen is L^3/λ on the basis of qualification and one model atoms can only erode one cell. When the material is subject to atomic oxygen attack with fluence F, the number of model atom M can be expressed:

$$M = F\lambda W^2/W_d \quad (1)$$

For narrow defect (see Fig. 4), the number of model atoms represented by true space fluence N is calculated [25]

$$N = \frac{M}{H}\frac{\lambda F}{DL}W \quad (2)$$

where N is the number of model atoms needed to simulated an effective fluence F for narrow defect (atoms), M is the number of model atoms for width defect, where defect width is greater than polymer thickness, λ is the reaction coefficient(cm/atom), W is the narrow crack width (cell), H is the width crack width (cell), D is