TECHNICAL SPECIFICATION

ISO/TS 22295

First edition
2021-05

Space environment (natural and artificial) — Modelling of space environment impact on nanostructured materials — General principles

Environnement spatial (naturel et artificiel) — Modélisation de l'impact de l'environnement spatial sur les matériaux nanostructurés — Principes généraux

Reference number
ISO/TS 22295:2021(E)

Contents

Page

Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights. Details of any patent rights identified during the development of the document will be in the Introduction and/or on the ISO list of patent declarations received (see www.iso.org/patents).

Any trade name used in this document is information given for the convenience of users and does not constitute an endorsement.

For an explanation of the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT), see www.iso.org/iso/foreword.html.

This document was prepared by Technical Committee ISO/TC 20, *Aircraft and space vehicles*, Subcommittee SC 14, *Space systems and operations*.

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

Introduction

In the near future nanomaterials and nanoelements will be widely applied in spacecraft and space engineering. Nanomaterials superiority in mechanical, thermal, electrical and optical properties over conventional materials will evidently inspire a wide range of applications in the next generation spacecraft intended for the long-term (~15 to 20 years) operation in near-Earth orbits and the automatic and manned interplanetary missions as well as in the construction of inhabited bases on the Moon.

The near-Earth's space is described as an extreme environment for materials due to high vacuum, space radiation, hot and cold plasma, micrometeoroids and space debris, temperature differences, etc. Existing experimental and theoretical data demonstrate that nanomaterials response to various space environment effects can differ substantially from the one of conventional bulk spacecraft materials. Therefore, it is necessary to determine the space environment components, critical for nanomaterials, and to develop novel methods of the mathematical and experimental simulation of the space environment impact on nanomaterials.

Modelling is a very important scientific tool for explaining various phenomena and predicting the behaviour of existing and designing materials under different conditions. In the case of nanotechnologies, modelling and simulations become even a more significant method of studying nanomaterials and processes in the nanoscale due to difficulties of observing and measuring many nanoscale phenomena experimentally. In computational nanotechnology, it is necessary to develop new integrated approaches for different length and time scales that enable explaining mechanisms of mesoscale phenomena and predicting emerging material macro-properties.

The changes in the materials properties, caused by the space environment impact, are determined with structural parameters and processes that are related to different spatial scales: from the size of atoms and molecules to the size of macroobjects. There are a variety of simulation methods but most of them can be applied only for a special space and time range/scale because of underlying approximations. To estimate the durability of nanostructured materials to the space environment impact it is necessary to investigate both fundamental effects of incident atom/particle interaction with nanosized structures within very short time intervals and resulting effects of material damage and changes in their properties, that can be observed at micro- and macroscale within much longer periods. Thus, in general case to study the whole set of elementary processes and resulting effects it is necessary to apply the multiscale simulation approach.

The main concept of this document is:

— for main space environment components to choose the most important space and time scales;

— for every scale to choose the most important physical and chemical processes that occur in nanostructured materials under the influence of the given space environment component and can be considered as elementary for the chosen scale;

— for every process to determine a method (or a group of methods) that can be used for their simulations under space environment conditions;

— for every chosen method to describe necessary and possible approximations as well as its limitation when used for simulation of the given process.

Space environment (natural and artificial) — Modelling of space environment impact on nanostructured materials — General principles

1 Scope

The document considers peculiarities of the space environment impact on a special kind of materials: nanostructured materials (i.e. materials with structured objects which size in at least one dimension lies within 1 nm to 100 nm) and specifies the methods of mathematical simulation of such processes. It emphasizes the necessity of applying multiscale simulation approach and does not include any special details concerning concrete materials, elements of spacecraft construction and equipment, etc.

This document provides the general description of the methodology of applying computer simulation methods which relate to different space and time scales to modelling processes occurring in nanostructured materials under the space environment impact.

The document can be applied as a reference document in spacecraft designing, forecasting the spacecraft lifetime, conducting ground-based tests, and analysing changes of material properties during operation.

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 10795, *Space systems — Programme management and quality — Vocabulary*

ISO 17851, *Space systems — Space environment simulation for material tests — General principles and criteria*

ISO/TS 18110, *Nanotechnologies — Vocabularies for science, technology and innovation indicators*

ISO/TS 80004-1, *Nanotechnologies — Vocabulary — Part 1: Core terms*

ISO/TS 80004-2, *Nanotechnologies — Vocabulary — Part 2: Nano-objects*

ISO/TS 80004-6, *Nanotechnologies — Vocabulary — Part 6: Nano-object characterization*

3 Terms and definitions and abbreviated terms

3.1 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 10795, ISO/TS 18110, ISO/TS 80004-1, ISO/TS 80004-2, ISO/TS 80004-6 and ISO 17851 apply.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at http://www.electropedia.org/

3.2 Abbreviated terms

AMD	accelerated molecular dynamics
CC	coupled cluster
CI	configuration interaction
DFT	density functional theory
DFTB	density functional based tight-binding
ESD	electrostatic discharge
HF	Hartree–Fock method
kMC	kinetic Monte Carlo
MC	Monte Carlo
MD	molecular dynamics
MP	Møller-Plesset perturbation theory
QM/MM	quantum mechanics – molecular mechanics
UV	ultraviolet radiation
VUV	vacuum ultraviolet radiation

4 Nanostructured materials

The peculiar properties of nanomaterials are determined by the presence in their structure of nanoobjects – particles or grains, fibres, platelets, etc. with at least one linear dimension in nanoscale (size range from approximately 1 nm to 100 nm)[1]–[5]. The lower boundary of this range approaches the size of atoms and molecules; and its upper one separates nanoobjects from microobjects.

The strong influence of the material nanostructure on its properties is caused by the so-called nanometre length scale effects which can be of classical and quantum nature. The nanoscale effects appear when the size of structural objects becomes comparable with a certain parameter of material which has a considerable influence on some physical-chemical processes in the matter and consequently on the material properties[1],[2]. A mean free path of charged particles, a diffusion length, etc. may be regarded as such a parameter in the case of classical length scale effects; and for quantum ones its role is usually played by the de Broglie wavelength.

Another parameter of nanostructures is called dimensionality; it corresponds to the number of dimensions that lie within the nanometre range, and is used for analysing the quantum confinement effects[1],[2]. According to this parameter, all objects may be divided into four groups:

— 3D-objects – bulk materials;

— 2D-objects – nanofilms, nanoplatlets;

— 1D-objects – nanofibres, nanotubes, nanorods, etc.;

— 0D-objects – nanoparticles, nanopores, nanocrystals, quantum dots, etc.

In a 3D-object, electrons can move freely in all three dimensions. In a film whose width is comparable with the de Broglie wavelength (2D-object), electrons move without restrictions only in the film plane, but in the perpendicular direction they are in a deep potential well; that's why 2D-objects are usually called quantum well. In 1D-objects, or quantum wires, two dimensions are comparable with the de

Broglie wavelength. If the electron movement is limited in three directions, a nanostructure becomes a 0D-object, or a quantum dot with discrete electronic states.

Due to nanosized scale effects, nanostructured materials acquire novel mechanical, thermal, electrical, magnetic and optic properties, which can surpass the properties of conventional bulk materials[1],[2],[6],[7]. Nanocomposites with nanoclays, nanotubes and various nanoparticles as fillers are one of the most promising materials for space applications. They may be used as light-weighted and strong structural materials as well as multi-functional and smart materials of general and specific applications, e.g. thermal stabilization, radiation shielding, electrostatic charge mitigation, protection of atomic oxygen influence and space debris impact[8].

Therefore, the creation of polymer nanocomposites with fillers of various shape and composition may play the pivotal role in spacecraft development and implementation of challenging space projects. Among possible fillers, the main attention is paid to carbon nanostructures: fullerenes, carbon nanotubes (CNT), graphene that represent particular allotropic forms of carbon[6],[7]. Due to superior mechanical properties, high electric and thermal conductivity of these nanostructures, one may develop various light-weighted and strong multifunctional nanocomposites. Of special interest are CNT structural analogues, boron nitride nanotubes (BNNTs), that are electrical insulators and in addition to excellent mechanical properties and high thermal stability possess high resistivity to oxidation[9],[10].

5 Main space environment components and processes

5.1 General

The space environment has a significant damaging effect on many materials, including nanostructured materials. During the flight, the spacecraft is influenced by a set of space environment components: electrons and high-energy ions, cold and hot space plasma, solar electromagnetic radiation, meteoroids and space debris, vacuum and other factors[11]–[18]. As a result of this impact, various physical and chemical processes take place in the materials and elements of the spacecraft equipment, leading to deterioration of their operational parameters. Depending on the nature of the processes triggered by the impact of the space environment, the changes in the properties of materials and equipment elements can have different time scales, be reversible or irreversible, and present a different degree of danger for on-board systems. To evaluate the potential effects of the space environment on material properties and the characteristics of spacecraft equipment, it is important to determine the combinations of the most significant factors in various areas of outer space. In this case it should be regarded as effects caused by the impact of individual components of the space environment, and their combined effect[12].

5.2 Space radiation

5.2.1 General

Ionizing radiations of the Earth's radiation belts are electron and proton flows with energies from several hundred eV to several hundred MeV[11]–[15]. As a result of different penetrability and energy, ionizing particles exert influence on all materials independent of their location, both on the exterior of spacecraft (coatings, blankets) and inside it. The dominant degradation mechanism depends on type of material, LET, type of ray, etc. Ionizing radiation breaks chemical bonds but in other cases may lead to cross-linking in polymers. These processes cause decomposition, embrittlement, colour change and darkening, change in electrical resistivity, mechanical strength degradation, etc. Wire insulator indicates decrease in breakdown voltage or cracks.

5.2.2 Special features of nanostructured materials response

Existing experimental and theoretical data demonstrate that nanostructured materials response to space radiation can differ substantially from that of conventional bulk spacecraft materials[19]–[24]. When an electron or ion with high energy interacts with a nanostructure, only a small amount of energy of the incident particle is imparted to it. Therefore, a nanostructured object is characterized by a small number of additional charge carriers or structural defects that appear due to the irradiation;

and their number is reduced with increasing incident particle energy, which is opposite to the situation in conventional materials.

The migration of structural defects and charges in nanostructures and conventional materials also differ: already at the stage of the ballistic cascade, the displaced atoms have more opportunities to leave a nanoobject due to its higher surface area to volume ratio as compared to the bulk material, which leads to a cascade slowdown within the nanostructure[21],[24]. In the conventional bulk materials, displaced atoms can freely reach the surface, causing the material to swell while leaving the vacancies behind. These point defects can aggregate, forming larger obstacles to dislocation motion and causing hardening and embrittlement[7]. In nanostructured materials which contain a large number of nanoscale grains, the grain boundaries can capture interstitials and then fire them back into the lattice to destroy any vacancy that comes within a few nanometres of the grain boundary[20]. Therefore, in nanostructured materials, which are characterized by the presence of large number of grain boundaries, there exists an efficient mechanism which implies that boundaries act as sinks for defects and prevents accumulation of radiation-induced defects within the grain. Controlling radiation-induced-defects via interfaces is considered to be the key factor in reducing the damage and imparting stability in certain nanomaterials under conditions where bulk materials exhibit void swelling and/or embrittlement[22],[23].

Thus, processes of formation of structural defects and charge carriers due to the ionizing radiation, as well as subsequent processes of carriers and defects migration and recombination, differ substantially in conventional bulk materials and nanostructured materials. The influence of these processes on the radiation damage of nanomaterials is ambiguous[19]–[22]. In addition, it is necessary to take into account that the relationship between the stability of nanostructures to the formation and accumulation of radiation defects and the radiation resistance of nanomaterials, determined by a change in their performance characteristics, can be very complicated[20],[21]. By now, there is no sufficiently complete and generally accepted description of the specific radiation effects in nanostructures and their effect on the properties of nanomaterials and spacecraft elements built on them.

Special features of nanostructured materials response to the space radiation:

— presence of grain boundaries or interfaces (nanocrystalline materials, nanocomposites) acting as sinks for defects;

— possibility to use structures and substances possessing enhanced radiation tolerance as fillers in nanocomposites;

— ability of defect healing and enhanced sputtering due to high aspect ratio (nanostructures).

5.3 Atomic oxygen of the Earth's upper atmosphere

5.3.1 General

Atomic oxygen (AO) space environment in low Earth orbits is very dangerous for polymeric materials. High translational energy of O atoms due to the spacecraft orbital velocity enhances their reactivity, so atomic oxygen is capable to break bonds in polymeric materials and create a thin oxidized layer on the surface of some metallic materials, resulting in polymer erosion and severe structural and/or optical properties deterioration.

In general, AO affects near-surface layers of materials, and the ram facing surface of the spacecraft suffers the highest AO fluence. However, oxygen atoms can be reflected and penetrate into covered area via multiple reflections.

Some metals like silver and osmium are rapidly oxidized when exposed to AO. In the case of polymers, the hyperthermal oxygen flux causes fragmentation of the polymer chains and formation of volatile species. As a result, a typical carpet-like relief is grown on the surface (buried regions and profile peaks). Its topology is specific to polymer type.

There are two main approaches to improve the durability of conventional polymeric materials to AO:

— thin surface coatings or ion implantation;

— embedding AO resistant fillers into polymeric matrices.

5.3.2 Special features of nanostructured materials

Nanostructured materials (nanocomposites) can possess a higher durability to AO if they consist of AO resistant nanosized fillers (e.g. Si-containing and metal oxide nanoparticles). Under AO exposure, on the nanocomposite surface forms a layer consisting of nanofillers and protecting underlying polymer layers against AO attack.

5.4 Hot magnetosphere plasma

5.4.1 General

Hot magnetosphere plasma consists of particles with an average kinetic energy of 10 eV to 10^5 eV and is located mainly at heights measured by tens of thousands of kilometres[11]–[14],[16]. Main processes induced by hot magnetosphere plasma are as follows:

— surface and internal charging;

— surface defect formation and sputtering (see 5.2).

Charging of spacecraft materials in hot magnetosphere plasma is the accumulation of electric charge on the external spacecraft surface. This accumulated charge can be distributed unevenly on the surface due to its low conductivity (so-called differential charging of the spacecraft surface).

The main consequence of spacecraft charging is electrostatic discharges (ESD), which create electromagnetic interference to the performance of on-board devices, and in some cases damage and destroy construction and equipment elements.

The phenomenon of charging is related to three groups of processes:

— leakage of electron and ion plasma currents to the spacecraft surface;

— exchange of charged particles between the spacecraft surface and the environment;

— redistribution of electric charges on the spacecraft surface.

The processes of the first group do not depend on properties of spacecraft materials.

The processes of the second groups imply the consideration of all types of secondary emission due to impacts of plasma electrons and ions incident to the surface as well as photoelectron emission induced by solar radiation. However, charging can lead to the appearance of high negative potential (up to several tens of kilovolts) of a certain construction element on the spacecraft and thereby initiate field emission from its surface. The intensity of this emission is closely related to the form and size of edges.

The redistribution of electric charges on the spacecraft surface (the third group) is the most important factor which reduces gradients of electric potential: tangential ones between different elements on the surface and normal ones between the charged surface of dielectric materials and the metallic frame. So to describe the charging effects in spacecraft materials, it is necessary to take into account the electric conductivity of different objects which is related closely to their electronic structure.

5.4.2 Special features of nanostructured materials response

Nanostructured materials consisting of non-conductive polymeric or ceramic matrices with conductive nanofillers (nanotubes, nanoparticles, nanosheets, etc.) possess high surface and volume electric conductivity under certain conditions, namely, high enough concentration of fillers and their good dispersion[1],[2],[6],[7]. Due to this important feature, their usage on the spacecraft surface can minimize negative ESD effects. However, it should be taken into account that embedding nanosized fillers into the polymer and ceramic matrices can lead to the deterioration of other properties that can be important for spacecraft operation (e.g. optic transparency[8]). Additionally, some nanostructures (e.g. CNT) are