ISO/TS 22295:2021 (E)

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

Contents

Foreword

Introduction

1 Scope

2 Normative references

3 Terms and definitions and abbreviated terms

3.1 Terms and definitions
3.2 Abbreviated terms

4 Nanostructured materials

5 Main space environment components and processes

5.1 General
5.2 Space radiation
5.2.1 General
5.2.2 Special features of nanostructured materials response
5.3 Atomic oxygen of the Earth's upper atmosphere
5.3.1 General
5.3.2 Special features of nanostructured materials
5.4 Hot magnetosphere plasma
5.4.1 General
5.4.2 Special features of nanostructured materials response
5.5 Heating, cooling and thermal cycling
5.5.1 General
5.5.2 Special features of nanostructured materials
5.6 Meteoroids and space debris
5.6.1 General
5.6.2 Special features of nanostructured materials
5.7 Solar UV and VUV radiation
5.7.1 General
5.7.2 Special features of nanostructured materials

6 Multiscale approach to simulation of space components impact on nanostructured materials

6.1 Multiscale simulation methods
6.1.1 General
6.1.2 Quantum (electronic) scale
6.1.2.1 Ab initio methods
6.1.2.2 Density functional theory method
6.1.2.3 Quantum Monte Carlo
6.1.2.4 Semi-empirical methods
6.1.2.5 Quantum mechanics – molecular mechanics
6.1.3 Atomistic scale (molecular dynamics and Monte Carlo)
6.1.4 Mesoscale
6.1.5 Macroscale (continuum methods)
6.2 Radiation damage modelling
6.2.1 General
6.2.2 Quantum scale
6.2.3 Atomistic scale
6.2.4 Mesoscale
6.2.5 Macroscale

6.3 Modelling of atomic oxygen impact
6.3.1 General
6.3.2 Quantum scale
6.3.3 Atomistic scale
6.3.4 Mesoscale
6.3.5 Macroscale
6.4 Modelling of charging effects
6.4.1 General
6.4.2 Quantum scale
6.4.3 Atomistic scale
6.4.4 Mesoscale
6.4.5 Macroscale
6.5 Modelling of heating/cooling and thermal cycling effects
6.5.1 General
6.5.2 Atomistic scale
6.5.3 Mesoscale
6.5.4 Macroscale
6.6 Modelling of meteoroids and space debris impact
6.6.1 General
6.6.2 Atomistic scale
6.6.3 Mesoscale
6.6.4 Macroscale
6.7 Modelling of solar UV and VUV radiation effects
6.7.1 General
6.7.2 Quantum scale

7 Outlook

Annex A (informative) Multiscale simulation methods: software for simulation in different space and time scales

A.1 General
A.2 Quantum scale
A.2.1 ABINIT
A.2.2 CP2K
A.2.3 CRYSTAL
A.2.4 Firefly
A.2.5 GAMESS
A.2.6 Gaussian
A.2.7 Molrpo
A.2.8 Quantum ESPRESSO
A.2.9 SIESTA
A.2.10 TURBOMOLE
A.2.11 VASP
A.2.12 WIEN2k
A.3 Atomistic scale
A.4 Multiscale suites
A.4.1 Materials Studio
A.4.2 NWChem

Page count: 29