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THE EFFECTS OF COSMIC RADIATION ON MATERIALS AND CHANGES TO THEIR ELECTRONIC STRUCTURE

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Abstract: *The study of electronic structure and the impact of radiation on materials has raised significant attention due to its implications across various scientific disciplines and industrial applications. Exposing materials to radiation affects their structure, making this research essential for space exploration, satellite technology, and the development of radiation-resistant materials and electronics. It is critical for ensuring the safety and reliability of missions. Proficiency in software tools and models has become indispensable for predicting these changes and creating computational models to assess the potential effects of high-dose radiation.*

ВЛИЯНИЕ НА КОСМИЧЕСКАТА РАДИАЦИЯ ВЪРХУ МАТЕРИАЛИТЕ И КАК ТЯ ПРОМЕНЯ ТЯХНАТА ЕЛЕКТРОННА СТРУКТУРА

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Ключови думи: *материалознание, кристални твърди вещества, космическа радиация, електронна структура, теория на плътност на разпределението, компютърни програми, софтуер, изчисления*

Резюме: *Изучаването на електронната структура и влиянието на радиацията върху материалите е от особено значение в редица научни дисциплини и индустриални приложения. Излагането на материали на радиация влияе на тяхната структура и изучаването му е фундаментално за космическото изследване, технологията на сателитите и разработката на материали и електроника, устойчиви на радиация. От съществено значение е и за гарантиране на безопасността и надеждността на мисиите. Владеенето на софтуерни инструменти и модели е необходимост за предвиждане на тези промени и създаване на компютърни модели за оценка на потенциалните влияния от високи дози радиация.*

Introduction

Space presents extreme environmental conditions, including vacuum, extreme temperatures, microgravity, and radiation. Materials used in space missions [1] must withstand these conditions to ensure the reliability and success of spacecraft and equipment and must maintain their properties and functionality over extended periods to ensure success during long and demanding missions.

- Materials must shield astronauts, spacecraft, and sensitive instruments from harmful radiation.
- For future space habitats on the Moon, Mars, or in orbit, materials are essential for construction, radiation shielding, and maintaining a habitable environment.
- Materials used in spacecraft and spacesuits must be biocompatible and not emit harmful substances that could affect astronaut health.
- Materials play a role in life support systems, food packaging, and habitat design.
- Analyzing materials for recyclability and reusability is essential for reducing waste and conserving resources during long-duration missions.

Understanding the Arrangement of Electrons

Understanding the electronic structure of atoms is fundamental to material science. It provides insights into how elements interact to form compounds, why certain substances conduct electricity, and the basis for the diversity of chemical reactions observed in the natural world.

The electronic structure of an atom refers to how its electrons are distributed in energy levels, orbitals, and shells. This arrangement is fundamental to understanding an element's chemical properties, bonding behavior, and reactivity. Electrons in an atom occupy specific energy levels (electron shells - designated by the letters K, L, M, etc.).

The electronic structure of solids refers to how electrons are distributed among the atoms within a solid material. When atoms form a solid, e.g. a crystal, atomic energy levels are transformed into energy zones/bands. Understanding the electronic structure is essential for predicting the electrical, thermal, and optical properties of materials. It plays a critical role in the design and development of electronic devices, semiconductors, and advanced materials for various applications, including electronics, photonics, and energy technologies. When many atoms come together to form a solid, their electron orbitals overlap, creating a new set of energy levels in energy bands.

In a solid material, such as a crystal lattice, the electronic structure is described using energy bands. They represent ranges of energy levels that electrons can occupy. The valence band is the lower-energy band in the electronic structure of a solid. Electrons in the valence band are bound to their respective atoms and are not free to move throughout the solid. Above the valence band is the conduction band, which contains higher-energy levels. Electrons in the conduction band have enough energy to move freely within the solid and contribute to electrical conductivity. The band gap, also known as the energy gap, is the energy range that separates the valence band from the conduction band.

In insulators and semiconductors, there is a significant band gap. Electrons in the valence band cannot easily transition to the conduction band because it would require them to acquire a substantial amount of energy. This results in limited electrical conductivity in insulators and variable conductivity in semiconductors. In metals, there is no band gap, which allows electrons to move freely in the crystal lattice, leading to high electrical conductivity.

Density of states (DOS) is a concept used in condensed matter physics to describe the distribution of energy states or energy levels within a material or a system which is essential for understanding the behavior of electrons in the material and its electronic properties. It provides information about the number of available quantum states within a given range of energy values. DOS doesn’t tell us how many of these states are actually occupied by electrons however. Taking this into account it’s not difficult to understand that the more the energy increases, the more space we would need for the electrons in the conduction band and the more the density of states increases.

The Fermi level represents the highest energy level in the conduction band that is occupied by electrons at absolute zero temperature. The position of the Fermi level relative to the energy bands determines whether a material is a conductor, semiconductor, or insulator and affects its electrical and thermal properties.

In semiconductor materials, the electronic properties can be tailored by intentionally introducing impurities through a process called doping. Doping can increase or decrease the number of charge carriers (electrons or holes) and modify the conductivity.

Cosmic Radiation

Radiation encompasses a broad spectrum of energy in the form of particles or waves. This spectrum includes electromagnetic radiation (e.g., gamma rays, X-rays, ultraviolet, visible light, and radio waves) and particle radiation (e.g., alpha and beta particles, neutrons). Different types of radiation carry varying levels of energy, and this energy can interact with the atoms and molecules within materials which can lead to ionization and excitation of atoms, causing electronic structure changes in materials. This can have significant effects on spacecraft, materials, and the health of astronauts. They can penetrate spacecraft walls, create defects, degrade mechanical properties, and introduce electronic traps.

Energy Transfer and Ionization

Ionizing radiation, such as gamma rays and X-rays, possesses sufficient energy to remove tightly bound electrons from atoms, creating charged particles (ions) and free electrons. This process is called ionization.

The creation of free electrons and ions within a material can significantly impact its energy states. These free charge carriers can affect the material's electrical conductivity, electronic band structure, and energy levels. In semiconductors and insulators, for instance, the introduction of free charge carriers can alter their electronic properties, making them more conductive.

Defect Formation

Radiation can also lead to the formation of defects within the crystal lattice of a material. These defects include vacancies (empty atomic sites), interstitials (extra atoms positioned between regular lattice sites), and dislocations (structural defects). These defects introduce energy states within the material's bandgap, affecting its electronic structure and energy levels and alters the the material's electrical conductivity and optical properties.

Band Structure Modifications

Intense radiation can induce changes in the electronic band structure. Radiation-induced modifications to the band structure can result in shifts in energy levels, alterations to the density of states (DOS), and even the creation of new energy bands or states within the bandgap.

In certain materials that are typically insulators, ionizing radiation can induce electrical conductivity by creating electron-hole pairs. This phenomenon can significantly alter the electronic properties of insulating materials, leading to unexpected electrical behavior.

Interestingly, some of the effects of radiation on materials can be reversed or partially recovered through a process known as annealing. When a material is exposed to heat or other forms of energy, radiation-induced defects may migrate or annihilate, potentially restoring some of the material's original electronic properties. Annealing is a crucial aspect of materials science when considering the long-term effects of radiation exposure.

Calculating the impact of radiation on a material

Radiation Type and Energy: Identify the type of radiation to which the material will be exposed. Determine the energy levels or wavelengths associated with the radiation.

Radiation Interaction with Matter: Understand how radiation interacts with matter. Ionizing radiation can ionize atoms or molecules. Non-ionizing radiation can excite electrons to higher energy levels.

Dose Calculation: Calculate the radiation dose, which quantifies the amount of energy deposited per unit mass of the material. The dose depends on factors like the radiation intensity and exposure time.

Radiation Effects on Electronic Properties: Calculate changes in electronic band structures, energy levels, and charge carrier concentrations due to radiation exposure.

Structural Changes: Employ computational methods (e.g., molecular dynamics simulations) to model and predict structural changes.

Radiation-Induced Defects: Calculate defect concentrations and their impact on mechanical and electrical properties.

Materials Modeling: Utilize computational modeling techniques, such as density functional theory (DFT), to simulate radiation effects on the electronic structure, band gap, and charge transport properties. Use Monte Carlo simulations or molecular dynamics to study radiation interactions at the atomic and molecular level.

Experimental Validation:

Perform experimental measurements and tests to validate computational predictions and assess the material's response to radiation under controlled conditions.

Long-Term Effects:

Evaluate the long-term effects of radiation exposure, as certain materials may experience cumulative damage over time.

Calculating the impact of radiation on a material is a complex task that often requires a combination of theoretical modeling, experimental characterization, and a deep understanding of the material's properties. The goal is to predict how radiation exposure will affect the material's performance and durability in various applications, including those in aerospace, nuclear power, healthcare, and electronics. Below in Fig. 1 and Fig. 2 you see an overview of different computational methods and their usage in publications.

Several tools can help us calculate the electronic properties using DFT. These are DFT software packages like Quantum ESPRESSO, VASP, or CASTEP, Vesta. For those who have more experience with programming languages like python could also utilize github projects or other free tools and APIs such as the onse from materialsproject.org or abinit.org.

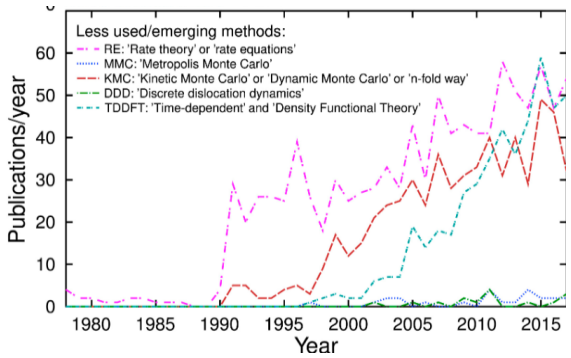

Fig. 1. Less used computational methods [2]

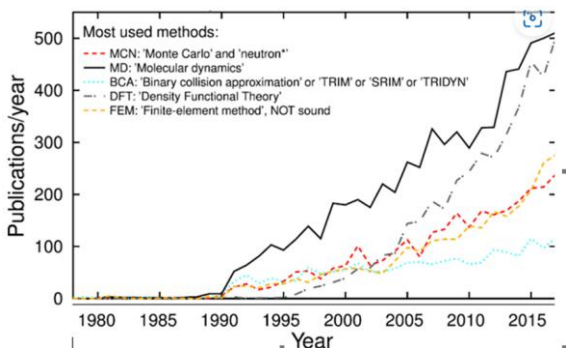

Fig. 2. Most used computational methods [2]

Computing DFT using Quantum Espresso (QE) [3, 4]

We will take a look at how we can use QE in order to do some basic calculations. Take into account that for more complex calculations you would need a supercomputer. Supercomputer System Avitohol exists and can be utilized at the IICT-BAS Institute of Bulgarian National Institute of Sciences.

For the purpose of the illustrations and experiments we will be using an Ubuntu virtual machine installed on a windows machine. As a material example we will use GaAs (Gallium arsenide) [5].
GaAs is a semiconductor compound used in some diodes, field-effect transistors (FETs), and integrated circuits (ICs).

1. **Preparing the environment.**

For the computational part we will make use of QE which runs on a Linux system.

Check on the Ubuntu website for instructions on how to install Ubuntu on a Windows Subsystem for Linux (WSL) on your local computer. You will have to enable a few windows features or install directly from powershell.

We will probably have to pre-install some packages such as gcc and fortran languages interpreter, ghostscript for .ps file conversions and python3-cif2cell for package input file conversions [6–9].

Once the Linux system is up and running we will proceed with the installation of the QE package via running the following command:

- sudo apt install quantum-espresso

2. **Prepare input file for calculations based on a crystallographic file.**

Download a so-called .cif file. A **Crystallographic Information File** (CIF) file, is a standard text-based file containing a common format to represent and exchange information about the crystal structure of materials, including their atomic coordinates and symmetry operations.

CIF files can be found on either of the websites: https://www.crystallography.net/ [10] or https://materialsproject.org [11].

We will make use of the python3-cif2cell package for Ubuntu and perform a transformation via the “cif2cell” command. This will generate the .in file which can be used as input for the Quantum espresso calculations.

- cif2cell GaAs.cif -p quantum-espresso -o gaas.in

Some modifications will need to take place on the gaas.in file based on **psuedopotential** files which can be found at the following location :

https://pseudopotentials.quantum-espresso.org/legacy_tables

Description of all fields of the input file can be found here: https://www.quantum-espresso.org/Doc/INPUT_PW.html

In order to avoid manual corrections you can directly use the generator provided by materials org: https://www.materialscloud.org/work/tools/qeinputgenerator [12–14]. This will directly generate a pw.*.in file format.

Below we can find an example input file where we used the Plane-Wave Self-Consistent Field (SCF) method for calculations [15]:

```
&CONTROL
  calculation = 'scf'
  prefix = 'GaAs'
  outdir = '.'
  pseudo_dir = '.'
  tprnfor = .true.
  tstress = .true.
  verbosity = 'high'
/
&system
ibrav = 2
celldm(1) = 10.6867
nat = 2
ntyp = 2
ecutwfc = 60
ecutrho = 244
/
&electrons
mixing_mode = 'plain'
mixing_beta = 0.7
conv_thr = 1.0d-8
/
ATOMIC_SPECIES
As     74.9216 As.pbe-n-rrkjus_psl.0.2.UPF
Ga     69.723 Ga.pbe-dn-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS
Ga 0.00 0.00 0.00
As 0.25 0.25 0.25
K_POINTS {automatic}
8 8 8 0 0 0
```

In order to perform the calculation execute the following command:

- pw.x -input gaas.in > gaas.out

Calculations produce an output file with information such as: total energies, Fermi level, kinetic energy cutoff, charge density cutoff, estimated scf accuracy, Cartesian and crystallographic axes, k-points, forces, information on highest occupied level including CPU usage and memory usage of the machine and many more.

This calculation is needed for further calculations and analyses of the band structure. We have to create a copy of the baas.in file and adapt some parameters such as the calculation method: calculation = 'bands', specify the number of bands: nbnd = 16 and specify K-Point configurations.

Execute the following commands:

- pw.x -input baasbands.in > baasbands.out
- bands.x -input baasbandsout.in > baasbandsout.out

In order to plot the bands use the following commands:

- plotband.x

```
Input file > GaAs.band
Reading   16 bands at     91 k-points
Range:   -8.1820   21.0070eV  Emin, Emax, [firstk, lastk] > -9, 22
high-symmetry point:  0.5000 0.5000 0.5000   x coordinate   0.0000
high-symmetry point:  0.0000 0.0000 0.0000   x coordinate   0.8660
high-symmetry point:  1.0000 0.0000 0.0000   x coordinate   1.8660
high-symmetry point:  1.0500-0.3000 0.3000   x coordinate   2.2932
high-symmetry point:  1.0000-1.0000 1.0000   x coordinate   3.2844
output file (gnuplot/xmgr) > gnumplot
bands in gnuplot/xmgr format written to file gnumplot
output file (ps) > gaasband.ps
Efermi > 6
deltaE, reference E (for tics) 5 0
bands in PostScript format written to file gaasband.ps
```

- ps2pdf gaasband.ps

This will produce a pdf file with the following information: see Fig. 3.

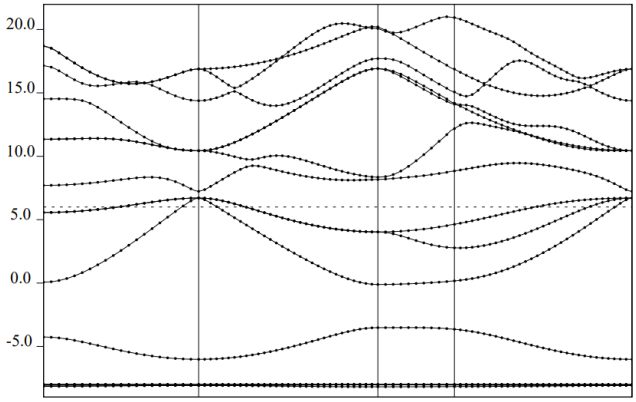

Fig 3. E (k) diagram; energy band structure of GaAs

Conclusion

We have reviewed only a small part of an existing simulation method in modelling radiation effects with QE. Many more DFT, MD and KMC methods exist and are advancing along with existing computational tools. It is worth investing collaboration and examining these tools further in order to determine if they are extendible enough. All of the methods will clearly remain in use for a long term to come.

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