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Research Article

Computer simulation of atomic structure of amorphous solids

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Abstract

This work is aimed at investigating the atomic structure of amorphous solids through computer simulations. Amorphous, solids, unlike crystalline materials lack long-range translational order or periodicity characteristics of crystals. With the growing computing capabilities and hardware improvements, computer simulation provides an alternate route to probe the amorphous nature of materials in an effective manner. Also, some of the computer simulating techniques employed in this work includes, the molecular dynamics, activation relaxation, and Monte Carlo based methods. This work also covers the applications and role of computer simulations.

Keyword: Computer, Atomic structure, Amorphous solids

INTRODUCTION

Computer simulation was developed hand in hand with the rapid growth of the computer following its first range-scale deployment during the Manhattan project in World War II to model the process of nuclear detonation. Computer simulation is often used as an adjunct or substitution for modeling systems for which simple closed form analytic solutions are not possible. Computer simulation provides an alternative route to probe the amorphous nature of materials in an effective manner. Therefore, computer simulation is the discipline of an actual or theoretical physical system, executing the model on a digital computer and analyzing the execution output.

To learn about the system we must first build a model of some sort and then operate the model.

Computer simulation is used to study the dynamic behavior of objects or systems in response to conditions that cannot be easily or safely applied in real life. For example a nuclear blast can be described by a mathematical model that incorporates such variable as heat, velocity and radioactive emissions.

Additional mathematical equations can then be used to adjust the model to change in certain variables such as the amount of fissionable material that produced the blast simulation are especially useful in enabling observers to measure and predicts how the functioning of an entire systems may be affected by altering individual computer within that systems.

AIMS AND OBJECTIVES

Computer simulation is useful when you need to see how a system will react to some changes in it, many times you cannot experiment with the real system so you have to model it and do a simulation over that model.

Computer Simulation models long-lived structural effort of ultraviolet irradiation on Computer simulation models the Physics of energetic fullerene projectile penetration, damage creation, sputtering and investigation in organic solids.

Computer simulation ascertains the response sensitivity characteristics in amorphous materials.

Computer Simulation is also used for example, in industry for improving the manufacturing process; in ecological and environmental sciences; for analysis of biodiversity and prediction of weather, ocean circulation, effects of deforestation, global warming etc. Also in social sciences for developing strategies for sustainable development and understanding social and economic change. Computer simulation studies the dynamic behaviour of objects or systems in response to conditions that cannot be easily or safely applied in real life. Computer Simulation aims at providing insight into the atomic structure of disordered solids

Primary sub-field of simulations

The primary sub-fields of simulation are; the model design, model execution and model analysis. To simulate something physically, you will first need to create a mathematical model, which represents that physical object. Models can take many forms including declarative, functional constant, spatial or multi-model. Once, a model is developed the next task is to execute the model on a computer, that is, you need to create a computer program which steps through time while updating the state and event variables in your mathematical model. The different ways to stop through time include, first leaping through time using event scheduling or employing small time increment using time slicing.

Also you can simulate the program on a massively parallel computer. This is called a parallel and distributive simulation.

For many large-scale models, this is the only feasible way of getting answers back on a reasonable amount of time.

The model

A computer simulation or a computational model is a computer program or network of computer that attempts to simulate an abstract model of a particular system. Computer simulations have become a useful part of mathematical modeling of many natural systems in physics (computational physics), chemistry and biology, human systems in economics, psychology, social science and in the process of engineering new technology to gain insight into the operation of those systems to observe their behaviour.

Computer simulation varies from computer programs that run a few minutes, to network based groups of computers running for hours, to ongoing simulation that run for days. The scale of event being simulated by computer simulations has far exceeded any thing possible (or perhaps even imaginable using the traditional paper-and-pencil mathematical modeling of 66,239 tanks, trucks and other vehicle on simulated terrain around Kuwait, using multiple supercomputers in the high performance computer modernization program; a 1billion atom model of material deformation 2002, a 2.64-million atom model of the complex maker of protein in all organisms, a ribosome, in 2005, and the Blue brain project at (Switzerland) began in May 2005, to create the first computer simulation of the entire human brain, right down to the molecular level.

A disordered material can be defined as one, which does not exhibit the long-range translational order of periodic characteristic of crystals. Such materials could be either solid or liquid, and this distinction is one time scale. Here, only solids are considered. A material is considered a solid when it is rigid; i.e. it does not flow when subject to moderate forces. A common criterion for rigidity is when the shear viscosity exceeds ns=$10^{13.6}$ Nsm^{-2}. These solids are also referred to as non-crystalline solids or glasses. There are various techniques used in simulating amorphous materials. Although the various features are very different, they share one common feature namely: a potential energy function to describe the atomic interaction.

Interaction potential

In principle any material structure can be obtained from the quantum mechanical Schrondinger equation. Solving the Schrondinger equation for an entire solid presents an enormous computational task and is not practical for our purposes, a number of approximations have to be made. Fortunately, the problem of modeling atomic structure is simplified because the mass of the electrons is much smaller than that of the nucleus while forces exerted on both are similar.

As a result, the motion of the atomic nuclei is much slower than that of electrons. This justifies the use of the Born-Oppenhenmer approximation. Only very light nuclei (such as hydrogen) or nuclear vibrations with frequency (w) which is such that hw>kbt, where h=the reduced plank constant and Kb=Boltzman constant. Also, within the classical description, the evolution of a system of particles follows from Lagrangian, L=K-V where K and V are the total kinetic energy and total potential difference of the system respectively. The P.E function is thus, a vital ingredient of every computer simulation because it is a function of the position of the particles, containing the information regarding the atomic structure. For amorphous solids, choosing the most suitable potential is a delicate matter. The consideration to be made is usually one of speed versus accuracy. The higher the accuracy of the potential, the more time is required to compute it.

Empirical potentials

These are the most common. They are not designed to describe the atomic bonding properties. The empirical potentials are computationally cheap to evaluate, hence very attractive for simulation involving many particles.

Finally, it is noted that computer simulations can be a powerful tool in unraveling the structure of amorphous materials.

Electronic properties

Theory for the electronic properties of crystals is greatly simplified by the lattice periodicity of such systems. In this case, the electron states can be written as Block waves, which extend through the entire crystals. The interaction between the electrons and the atomic cores situated at each lattice site gives to a number of band gaps. The band gap structure is important because it determines whether the crystal is a conductor or an insulator.

In amorphous materials the electron states cannot be written as Block waves because periodicity is absent. Analogous to lattice vibrations, a valid quantity to describe the electronic density of state (EDOS).

Short range order

While amorphous materials do not show the regular, periodic structure of crystals, they are by no means random. In many cases, the structure is governed by strict rules, especially on small scales. For example, amorphous silicon consists mostly of four-fold coordinated silicon atoms and the Si-Si bond length and the Si-Si-Si bond angle are close to the crystalline values of 2.35 Å and 109.47 degrees, respectively.

The presence of short-range order is illustrated with the radial distributions function (RDF). The RDF g(r) is the local number of identity of atoms at a distance r from a reference atom, averaged with respect to the choice of this atom. At larger distance, the RDF tends to a Constance value, which indicates disorder.

In retrospect, amorphous materials are not random but contains some degree of short range order. In contrast to crystalline materials, long-range order is absent. The absence of long-range order in amorphous materials turns out to have dramatic effect on their vibrational properties.

Vibrational properties

Atomic vibrations in a solid have a profound effect on its properties. For example heat is transported through atomic vibrations and the specific heat of materials is determined mostly by the spectrum of allowed vibrational modes.

Furthermore, under certain conditions, electromagnetic radiation can interact with atomic vibration (for example in Raman scattering) thereby directly determining the optical properties of the material. In crystals, vibrational modes can be classified in terms of the wave vector because of lattice periodicity. This gives rise to a number of dispersion relations, which describe the dependence of the vibrational frequency on the wave vector. For amorphous solids this classification is not possible. Vibrations in this case are usually described in terms of vibrational density of states or VDOS.

This suggests that short-range order (which is the same in both the crystalline and the amorphous forms) determines the vibrational properties. The short-range order directly influences the shape of the VDOS. In other words, the VDOS can be used to probe the structure of amorphous materials in experiments.

PREPARATION OF AMORPHOUS SOLID

Melt-quenching

The oldest method of producing an amorphous solid is to cool the molten form of the material sufficiently quickly. This process is called melt quenching. Amorphous materials produced in this way are often called glasses because many such materials show a glass transition, through not all.

This naming convention has been the source of confusion for many years.

When a liquid is cooled, either a crystal will form or an amorphous solid is formed by the continuous hardening (increase in viscosity) of the melt as a whole. An essential criterion for producing amorphous materials is therefore that the cooling process be fast enough to preclude crystal growth. The crystal phase is thermodynamically more stable and will dominate if allowed to take place. Therefore, the cooling rate is a critical factor in the production of amorphous solids

Identification of Vacancies and Interstitials In Amorphous Solids

Vacancies can be defined as the missing electron in the crystal structure.

Some vacancies have been identified such as lattice vacancies, isolated vacancies and unrelaxed vacancies. A Great deal has been learned about lattice vacancies and their interactions with other defects.

The lattice vacancy is a soft, polarizeable defect, which, each time you add an electron can relax in such a way as to keep electrons apart and minimize their columbic repulsion.

Isolated vacancies have been identified, as have divacancies and higher aggregate of vacancies. The energy for unrelaxed vacancies are found to be increasing with electronic charge due coulomb repulsion between the highly localized electrons. Allowing the vacancies relax for each charge state, however lowers their corresponding level and compresses them together.

In a theoretical treatment of the vacancy, it is absolutely essential to include distortions as an integral part of the model because of the electrical level position and wave function of the defect level and the importance or not of many electrons.

A large number of vacancy- impurity pairs have also been identified. For all, simple one-electron molecular orbital models made up from the dangling broken bonds around the vacancy serve to satisfactory describe their electron structure.

Interstitials on the other hand, is said to be the spaces that exist between 3-D crystal structures.

Isolated interstitials, a wide variety of interstitial- impurity pairs and possibly di-interstitials have been observed. For many of these interstitialcy, bonded configurations are observed consistence with the theoretical predictions based upon molecular orbital calculations of finites atom clusters.

Neither the isolated interstitial nor the vacancy is stable at room temperature and they therefore are encountered at room temperature only in trapped or aggregated states.

Computer simulation techniques

The three basic techniques used in simulating amorphous material are; molecular dynamics, the activation-relation Monte Carlo based method. Although the various techniques are very different, they share one common feature namely: a potential energy function to describe the atomic interaction.

Molecular Dynamics Method

Molecular dynamic method of computer simulation is used to study vacancies and interstitials in one component amorphous solid, where the atomic interaction are described by a Lennard-Jones pair potential. In the beginning of a computer experiment, a defect is introduced into a sample by removing or adding and atom and after relaxation the properties of the defect are monitored by different probes, for vacancies, cavity analysis is applied where one determines the empty space inside the material. The interstitials are identified by computing the local atomic pressure, which for interstitials differ markedly from the pressure distribution of non-interstitial atoms.

Molecular dynamics is a form of computer simulation in which atoms and molecules are allowed to interact for a period of time by approximation of known physics, given a view of the motion of the atoms. Because molecular systems generally consist of a vast number of particles, it is impossible to find the properties of such complex systems analytically. When the numbers of bodies are more than two no analytical solutions can be found and result in chaotic motion. Molecular dynamics simulation represents an interface between laboratory experiments and theory and can be understood as a “virtual experiment”

Activation Relaxation Method

Activation relaxation method efficiently identifies the relevant diffusion mechanism in a wide range of systems either crystalline or amorphous with both empirical and abinitio methods. Activation relaxation has been used for a number of applications ranging from the structural optimization of amorphous material to the identification of relaxation and diffusion mechanisms in complex materials. This approach was used to produce well relaxed configurations of disorder systems such as si and lennard Jonnes glasses.

Activation relaxation method is also an existing self-learning, off lattice kinetic Monte Carlo algorithm that opens the door to the numerical study of such as semi conductor growth, self organization, defect diffusion and interface mixing which have until now been out of reach of simulations. This method demonstrates that elastic deformations are determinant to the diffusion kinetics of vacancies.

Monte-Carlo Method

A Monte Carlo method is a technique that involves using random numbers and probability to solve problems. The term Monte Carlo method was coined by S.Ulam and Nicholas metropolis in reference to games of chance, a popular attraction in Monte Carlo, Monaco. Monte-Carlo simulation is a method for effectively evaluating a deterministic model using set of random numbers as inputs. This method is often used when the model is complex, non linear or involves more than just a couple uncertain parameters. In Monte-Carlo simulation the time scale is determined by the fastest activated processes. Though, Monte Carlo method has been extensively and successfully used over the past 20 years, it suffers from a number of drawbacks. In particular, the systems investigated must be discretized and mapped onto a fixed lattice in other to define the various diffusion mechanisms that need to be considered at given moment. Once all processes on the lattice have been identified, the simulation simply consist in operating a diffusion event picked at random, updating the list of possible moves in the new configuration and interacting this procedure long enough to cover the relevant physical time scales. This approach works very well for simple problems (e.g., surface diffusion, metal-on-metal growth) but fails when the systems undergo significant lattice deformations or when long-rang elastic effects are important.

The role of computer simulation

Clearly, the construction of large high quality CRNs by hand is not practical. Nowadays, the generation of CRNs is carried out on computers. In this case, atoms on the edge of the simulation volume interact with atoms on the opposite edge and vice versa. This way there are no special surface atoms, which have different properties from the others.

The first computer-generated networks, which date back to the sixties and seventies, typically contained a few hundred parties. More advance algorithms and faster computers have increased the size of the networks that can be handled to a few thousand atoms, with simulation cells of up to 40x40x40 Å^3 .As the simulation cells increase in size, actual devices decreases in size. In certain solar cells, the thickness of the amorphous silicon layer (which forms the bulk of the cell) can be as low as 1000 Å. To model this layer one could use periodic boundary conditions in two extended directions. In these directions, a length scale of 30 Å is sufficient to capture the randomness of the material.

A reasonable model of the layer would thus require a simulation volume of 30x30x1000 Å^3, containing approximately 45, 000 atoms. Well-related network of this size are currently able to generate by using a highly optimized algorithm. This achievement paves the way for the generation of realistic device-size atomic networks

An exciting application of this network would be the simultaneous of an entire electronic device (such as a solar cell or a transistor) at the atomic level.

CONCLUSION

Computer simulation has become a useful part of mathematical modeling especially in computational physics to gain insight into the operation of those systems to observe their behaviour. The atomic structure of amorphous solids is investigated through computer simulation because experimental techniques alone are not sufficient to determine their structure.

As a result, computer simulation is an essential tool in the identification of vacancies and interstitial is in amorphous solids. Thus, it probes the amorphous nature materials in an effective manner.

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