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Study of crater formation and its characteristics due to impact of a cluster projectile on a metal surface by molecular dynamics approach

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ABSTRACT

Impingement of energetic particles/ions on material surfaces is of great interest as these impacts give rise to various interesting phenomena, such as sputtering, back-scattering, crater formation, emission of electrons and photons from material surfaces etc. Surface erosion occurring in the plasma-facing material of nuclear fusion reactors reduce their performance and this motivated the course of the current work in understanding the underlying physics of solid–particle interactions. In the present work, we have studied sputtering, crater formation and its characteristics on the surface of a plasma-facing material due to the impact of a low to high energy dust particle (a conglomerate of a few to a thousand atoms) using the molecular dynamics method. Sputtering yield, excavated atoms from the crater, crater depth, height of crater rim, radius and aspect ratio of the crater are calculated for a range of incident energies (10 eV to 10 keV), and the variation of these parameters with varying size (formed of 14, 32, 64 atoms) of dust particle at different temperatures of the target material are computed.

1. Introduction

An abrupt increase in the demand of world energy consumption due to rapid industrialization and objections on the use of fossil fuels concerning environmental issues made the researchers focus on an alternate source of energy to meet the ardent need. Though the renewable energy is eco-friendly, there is no assurance that this energy can fulfill the future need. Thermonuclear fusion comes out as an alternate source of energy, which is examined to be environmentally friendly and safe, where light nuclei fuse to form a heavy nucleus releasing a tremendous amount of energy [1]. After decades of momentous research on making use of thermo-nuclear fusion for energy production, construction of International Thermonuclear Experimental Reactor (ITER) [1] is a witness of usability of thermonuclear fusion energy for commercial purposes. Although ITER reached a demonstrative phase, there are a lot of challenges to overcome. One of the challenges faced by ITER is the choice of plasma-facing material (PFM), which can withstand tremendous energy from fusion reaction and impact of dust particles on PFM. Tungsten (W) is considered as one of the potential materials for PFM over other materials due to its high melting temperature (3683 K) and low erosion rate because of its high atomic number ($Z = 74$)[2].

It is evident that small particles of dust are ubiquitous in plasma of nuclear fusion reactors [3]. These dust particles are produced due to the interactions between plasma and material-surface in a nuclear fusion reactor through mechanisms like blistering [4], flaking, melting, arcing and sputtering. The dust particles thus produced can contaminate the plasma and affect the performance of a reactor. Interaction of dust and PFM has an effect on the operational life of PFM. Also, the presence of dust particles can pose a serious threat to the safety of the fusion reactors [3].

When the surface of a target material is bombarded with energetic particles, it gets eroded as surface atoms are removed and the morphology of the surface gets modified. This phenomenon on the atomic scale is usually called "*Sputtering*". Thus, sputtering is the ejection of particles from the surface of a solid target material due to impingement of high energy particle. It comes under the broad subject of solid–particle interaction. The incident particle may be a photon, an electron, an ion, or a clustered projectile of atoms (the one considered in this work). Sputtering occurs as the result of a series of elastic collisions where momentum transfer takes place from incident energetic particles to the target atoms within a collision cascade region. A surface atom of the target material ejects as a sputtered atom if it receives a component of kinetic energy normal to the surface of the material that is sufficient to overcome the surface binding energy (SBE) of the target material.

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Apart from sputtering, several other effects may also be observed due to particle bombardment of material surface, depending upon the kind of interaction involved between energetic particles and the atoms of surface material. A fraction of incident particles back-scatter in collisions with target atoms, the others get implanted in the material and come to rest inside the solid in transferring their energy to target atoms. The particle bombardment may also cause emission of electrons, photons and, finally radiation damage in the surface layers of the solid, i.e., a change of the surface structure and topography etc.

As mentioned before, sputtering is known to be a phenomenon occurring on the atomic scale. However, after bombardment with a large number of particles, macroscopic effects such as change in weight of the material may be observed, and crater may be observed on the target material facing the incoming energetic particles. The sputtering phenomenon was first discovered more than a century ago in 1852 as the erosion of cathode in electric gas discharge tube by Grove [5] and was named "cathode sputtering". Goldstein [6] in his ion-beam sputtering experiment, demonstrated the disappearance of a gold coating on a glass wall facing the beam and presented evidence that sputtering was caused by positive ions of the discharge hitting the cathode. Although progress in understanding the sputtering phenomenon was sluggish, possible uses of the phenomenon were recognized early. The potential of the sputtering phenomenon in thin-film coating was mentioned by Plücker [7]. It took about 100 years until the physical processes involved in sputtering were clearly understood, and about another 20 years until a quantitative description of the sputtering process had been developed. The field started developing rapidly since 1950, but several important aspects are still under active investigation today.

Merkle and Jäger [8] used transmission electron microscopy to study the formation of surface craters by bombarding thin Au foils of thickness 60–80 nm with Bi^{+} and Bi_2^{+} in the incident energy range of 10–500 keV. It was found that the size of the crater was considerably smaller than the cascade size, and also noticed that around 2000 atoms have been excavated from crater of diameter 5 nm. The authors also found that craters were formed in individual displacement cascades. In another study using the transmission electron microscopy, Birtcher and Donnelly [9] observed holes on thin Au foils when bombarded with 200 keV Xe ions. It was found that the holes had diameters between 5 and 10 nm. The authors also observed that the holes were formed in the regions where the thickness was about 50 nm and more, from which they analyzed that the average cascade had a vertical dimension of at most 50 nm. In yet another work of Donnelly and Birtcher [10], while investigating irradiation of Au films with Xe ions in the energy range 50–400 keV, they observed the formation of crater and annihilation.

Solid–particle interactions have been an area where the simulation studies started earlier than in many other fields. Reasons were likely the need to model stochastic processes and such studies do not necessarily need quantum mechanics. The two main methods used for the simulation of ion bombardment of solids are the classical molecular dynamics method [11], and the Monte–Carlo approach using binary collision approximation [12]. The first computer simulation of movement of atoms of a small crystalline structure using the former approach dates back to a publication of Alder and Wainwright [13]. The application of computer simulation to investigate radiation damage by using the classical molecular dynamics method by Gibson et al. [14] opened a wide new field. At about the same time, Monte–Carlo simulations using the binary collision approximation were started by Bredov et al. [15] to study penetration and by Goldman et al. [12] to study sputtering.

Sputtering is a phenomenon in which resolving the interaction of high energy particle with a surface is of utmost importance. The time scale associated with each impact of high energy particle on a plasma facing surface is such that the entire sputtering process gets over within a few picoseconds. Only molecular dynamics approach can truly replicate the phenomenon occurring at such small time and length scales. Understanding the sputtering phenomenon at the atomistic level may help us make an assessment of the probable life of the plasma facing surfaces used in thermonuclear fusion reactors. Therefore, in this work, we would focus on the molecular dynamics approach of investigation of the problem of sputtering of surfaces by impingement of high energy particles.

Using the classical molecular dynamics method, Bringa et al. [16] investigated the formation of craters during 0.4–100 keV Xe bombardment of Au. The authors observed craters and associated rims, ad-atoms and sputtered atoms. The authors concluded that sputtering mechanism can not be understood on single parameter i.e., energy density. In low energy regime, the formation of crater was due to the cascades of high energy density and in high energy regime, formation of crater and its rim was due to liquid flow of atoms, which was created in the thermal spike and forced onto the surface due to high pressure.

Smith et al. [17] carried out molecular dynamics simulations of the bombardment of C_{60} on graphite and silicon crystal surfaces. The authors have found that for incident energies up to 450 eV, normally incident C_{60} generally reflects intact from the graphite surface causing hexagonal waves to propagate from the impact point. At 1 keV, the molecule compresses and implants into the graphite structure. Up to 6 keV, little sputtering was observed and at 15 keV, sputtering yield increases and surface ruptures near the impact point. For silicon case, it was observed that at higher energies, larger craters were formed with higher sputtering yield.

Yang and Hassanein [18] examined the behaviour of tungsten as plasma facing material by investigating the erosion and surface evolution of tungsten material using the molecular dynamics method. The authors studied the carbon trapping rate, implantation depth and sputtering yield of tungsten due to the bombardment of deuterium and carbon ions at varying energies. To understand the dust and plasma facing material interaction Guo-jian Niu et al. [19] investigated the evolution of kinetic energy, potential energy and total energy of the tungsten based plasma facing material bombarded with tungsten dust particle consists of 541 atoms with energies 1, 10 and 100 keV/dust particle. In the present work, we have investigated crater formation on a tungsten plasma facing material and its sputtering characteristics by bombarding it with tungsten dust/cluster particles of three different sizes (formed of 14, 32, 64 atoms) at varying energies ranging from 0.01–10 keV/dust particle. Tungsten only is studied in this study as the plasma facing material, since it is the most widely used material in nuclear reactors [18]. Characteristics of surface due to impact of high energy particles are studied using properties such as radius, depth, aspect ratio of carter formed on surface, sputtering yield etc. Understanding on these aspects can help in designing surfaces for systems involving impact of high energy particles. Such a study is not carried out so far to the best of the knowledge of the authors. Thus the present study sheds light on the details of sputtering characteristics of a plasma facing material, which can be of interest to the readers, and can help in designing suitable surfaces for specific applications. For example, the approach developed here can also be used to analyze the mechanical erosion of nozzles in a solid rocket motor, in which the impact of aluminum/alumina particles on