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Melting and shock wave creation in uranium oxide due to Coulomb explosion after a pulsed ionization

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ABSTRACT

By means of molecular dynamics simulations, we study the effects of pulsed ionization in uranium oxide (UO_2), which occurs when UO_2 is bombarded with swift ions or fission fragments. A general formula is developed to predict melting radius under various conditions due to electron stripping and Coulomb explosion (CE). A critical density model is suggested in which the melting volume is proportional to ionization period, if the period is above a critical value. The maximum melting radius depends on the time period of structural relaxation above the melting temperature, which increases with increasing initial substrate temperatures due to a lower heat dissipation rate. Furthermore, shock waves are observed to emit from CE core but the kinetic energy wave peak exists only in U sublattices. The absence of kinetic energy waves in O sublattices is explained by their relatively higher thermal vibration which cancels the work done from the compression waves.

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1. Introduction

In numerous previous studies, it has been observed that swift ions can create ion tracks in insulators, semiconductors, and polymers. The fundamental mechanisms of track formation, however, are still subject to some debate [1–5]. Coulomb explosion (CE) and thermal spike model were often compared as competing mechanisms. Bringa and Johnson supported CE mechanism [1], while many other studies favored thermal spike model [2–5]. In the thermal spike model, energetic electrons are created under a high electron stopping power and subsequent electron-lattice coupling leads to melting and lattice disorders [6–8]. In the CE model, swift ions cause strong electron ionization of target atoms, leading to partial electron depletion along an ion track. In semiconducting or insulating substrates, the lack of free electrons makes it difficult to quickly recover the charge neutrality through electron back diffusion. With an ionization period sufficiently long (>a few fs), Coulomb force among the positively charged target atoms lead to CE [9], through the following stages: first, Coulomb potentials quickly convert to kinetic energies of atoms during the ionization pulse. Second, within a factor of 1 ps, kinetic energies are shared among atoms and local thermal equilibrium is reached. This process also leads to local melting. Third, the melting zones are cooled down and form either amorphous or polycrystalline cores, depending on rates of heat dissipation to the surrounding medium.

Swift ion induced ion track formations can be used in microtechnology and nanotechnology for a wide range of applications [10–12]. Ion track formation in uranium oxide (UO_2) is particular important for light water reactors, due to the facts that fission fragments from neutron reactions, in a typical kinetic energy of 100 MeV, may lead to structural changes which cause thermal and mechanical property degradation, and influence reactor performance. Experiments on both accelerator based swift ion irradiations and reactor irradiation have observed ion track formation in UO_2 [13,14]. Computer simulations have been used to understand CE effects [15–18]. In the present study, we preformed systematic molecular dynamics (MD) simulations, in order to understand CE mechanism. Many previous studies have used MD simulations to understand thermal spike model. Modeling studies on CE phenomenon, however, are very limited. The present study has no intention to evaluate the competing effects between Coulomb explosion model and thermal spike model, but expect to benefit the development of a comprehensive model to possibly combine both effects.

2. Modeling procedure

The present study is aimed to understand atomic scale details of CE in UO_2, and to identity key parameters which influence the

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microstructure changes after CE. Instead of directly linking the modeling to specific fission production irradiation, CE is introduced by a pulsed ionization. The ionization time period and the substrate temperatures are used as variables for systematic investigation. Another reason to introduce a pulsed ionization is to alleviate issues from molecular dynamics (MD) simulations. MD simulations cannot handle electron subsystems.

MD simulations are performed by using the LAMMPS (Large-scale Atomic Molecular Massively Parallel Simulator) code [19]. The interatomic potentials were described by a partly ionic Busing-Ida-type using potential parameters proposed by Yakub et al. [20]. Many interatomic potentials have been developed to describe UO_2, as reviewed by Govers et al. [21]. These potentials include the two major types [20]: one has charges fixed by the chemical compositions and the other, the Busing-Ida type [22,23], has fractional effective charges. Introducing effective charges provides an important fitting parameter to match with experimental observation. Most importantly, the potential used in the present study is able to accurately predict melting and existence of a pre-melting structural transition [20]. As to be discussed, the transition from solid to liquid is one important phenomenon introduced by CE. The used potentials include Coulomb interactions and short-range interactions. The short-range interactions consist of O–O van der Waals attractions, and U–O covalent bonding represented by the Morse function and overlap (exchange) repulsion.

The unit cell has a dimension of about 22 nm × 22 nm × 5.5 nm and contains 192,000 atoms. The cell is [100] oriented. All sides take periodic boundary conditions, including the top and the bottom of the cell. The geometry of the cell is schematically shown in Fig. 1. After thermal relaxation at 300 K for 50 ps, an ionization pulse was introduced in a cylindrical region of radius 20 Å. From 0 to 10 Å, half of the U and O atoms within the ionized region are stripped by one electron per atom, f.g. $U^{4+} \rightarrow U^{5+}$, to simulate CE. From 10 to 20 Å, the stripped electrons in the CE region are re-distributed, forming an electron rich cylindrical shell surrounding the electron-stripped core. These electrons are added to local U/O atoms so their Columbic force contributions are included in MD simulations. Without such treatment, charge neutrality cannot be preserved, and the accumulated electric fields from positively charged core are high enough to introduce significant Coulomb force and create abnormal cell vibrations. The approach of redistribution of stripped electrons near the CE core effectively creates charge screening effect to eliminate the long range Coulomb force from the core. At the end of the ionization, these redistributed negative charges, together with positive charges introduced in the CE core, are removed simultaneously under assumption of quick charge recovery.

For the present study, ionization period range from 5 fs to 10 fs. The time selections consider the facts that electron ionization, and electron–electron thermalization occur in a typical time scale of 1 fs [2]. Once the ionization pulse ends, the pair Coulomb potential was removed. For the rest of the discussion, the time $t = 0$ refers to the moment when the ionization starts. The cell is divided into cylindrical slabs and closest atomic separated distance (CSD) of each slab, based on the average value of the first neighbor distance within the slab, is extracted to plot CSD radial distributions. The melting radius can be quantitatively determined since CSD values of melting UO_2 are larger than that of amorphous UO_2. And both of them are larger than that of crystalline UO_2. It needs to point out that a defective crystalline UO_2 layer may create high CSD values but they are typically less than that of amorphous UO_2 and do not show saturation. For a local molten core surrounded by defective zones, radial CSD values are featured with a step height peak corresponding to the molten core and a decreasing tail corresponding to surrounding defective zone. Therefore, we use half height of

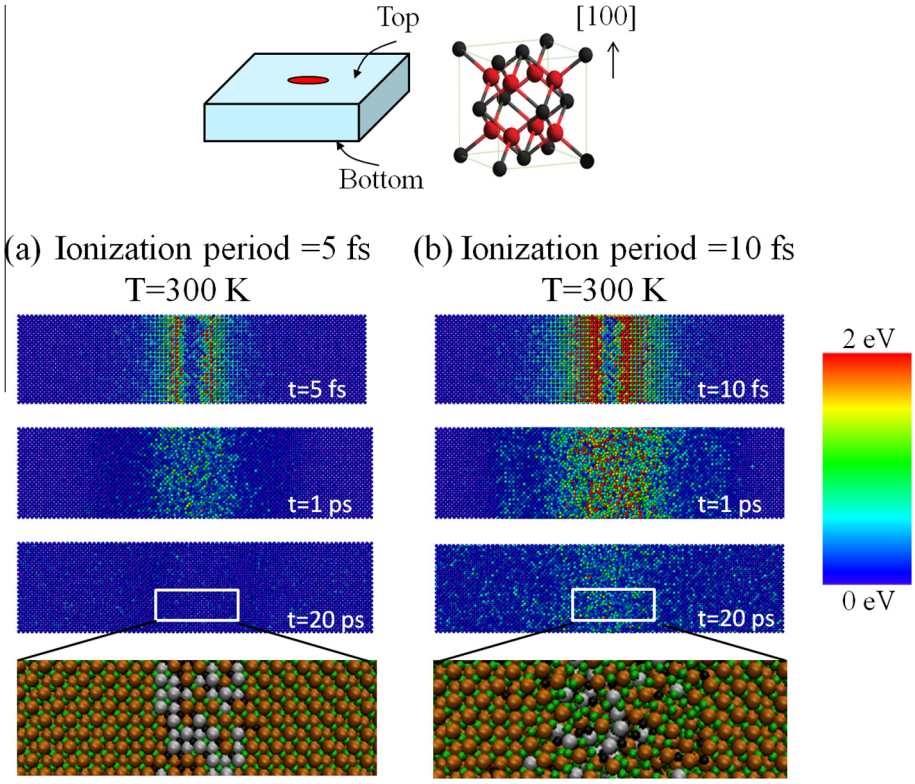

Fig. 1. Kinetic energy distributions in UO_2 for an ionization period of (a) 5 fs and (b) 10 fs. Ionization is introduced in the cylindrical region of 10 Å radius. The initial temperature is 300 K. The bottoms are enlarged images showing atom disorder levels. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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