



The role of electronic energy loss in ion beam modification of materials



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ABSTRACT

The interaction of energetic ions with solids results in energy loss to both atomic nuclei and electrons in the solid. In this article, recent advances in understanding and modeling the additive and competitive effects of nuclear and electronic energy loss on the response of materials to ion irradiation are reviewed. Experimental methods and large-scale atomistic simulations are used to study the separate and combined effects of nuclear and electronic energy loss on ion beam modification of materials. The results demonstrate that nuclear and electronic energy loss can lead to additive effects on irradiation damage production in some materials; while in other materials, the competitive effects of electronic energy loss leads to recovery of damage induced by elastic collision cascades. These results have significant implications for ion beam modification of materials, non-thermal recovery of ion implantation damage, and the response of materials to extreme radiation environments.

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1. Introduction

The use of energetic ion beams to synthesize and modify materials has evolved over the past several decades. Ion beam modification of materials employs energetic ions over a broad range of energies to controllably change electrical, optical, structural, mechanical and chemical properties of materials for a broad range of research and applications [1–5], including advanced electro-optical devices and engineered nanostructures. The interaction of ions with solids results in energy loss to both atomic nuclei and electrons in the solid. Energy transfer to the electronic and atomic structures, and corresponding response of materials, can be divided into three principal energy regimes. At low ion energies ($E < 0.5$ MeV), the transfer of energy to atomic nuclei (nuclear energy loss) dominates, leading to the displacement of atoms via elastic scattering collisions between atomic nuclei in ballistic collision cascades. For high energy ions exceeding ~ 1 MeV per nucleon (MeV/u), particularly for swift heavy ions ($E > 50$ MeV), electronic energy loss dominates, leading to intense local ionization that can cause damage production [6], track formation [7] or damage recovery [8], and the formation of long, straight ion tracks with nanometer diameters by swift heavy ions has been exploited in a

range of nanoscience applications [9,10]. At intermediate ion energies ($0.5 < E < 50$ MeV), nuclear and electronic energy losses are of similar magnitude, which can lead to additive effects on damage production [6,11] or competitive recovery processes [12–14] that affect damage accumulation and nanostructure evolution during ion beam modification.

While it is well established that the interaction of energetic electrons, ions and neutrons with solids initiates a cascade of energy transfer processes on both the electronic and atomic structures, irradiation effects research on materials has focused largely on the separate effects of energy transfer to the atomic structure for much of the past 50 years. Due to the complexity of the problem and the heretofore limitation of available experimental and computational tools, the dynamics of energy transfer to electrons and exchange of energy between electrons and ions/atoms are much less understood. In recent years, the importance of these ionization effects and the coupling of electronic and atomic processes has become increasingly recognized for both metals [15,16] and ceramics [12,14,17]. The development of radiation-tolerant materials and the control of ion beam modification methods to create defects and nanoscale structures that tailor materials properties or create new functionalities demand a comprehensive understanding and predictive models of energy transfer and exchange processes at the level of electrons and atoms.

This review focuses on recent advances in understanding and modeling the effects of energy loss to electrons on ion beam modification of materials, with particular emphasis on the intermediate

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energy regime from a few hundred keV to tens MeV. The effects and applications of swift heavy ions [18,19, this issue] and cluster ions [20, this issue] are covered in companion reviews, as are advanced techniques in characterization of ion beam modified materials [21, this issue]. We will first summarize the advances in computational approaches, and then present and discuss the response of materials to single ions, to the separate effects of nuclear and electronic energy loss, and the combined effects of dual ion-beam experiments.

2. Advances in computational methods

While there is a general understanding of the physics involved in the evolution of a single ion event, detailed predictive models are lacking. This is the most fundamental and critical source term in understanding and modeling the collective response of materials to ion irradiation over a broad range of ion energies and irradiation conditions. Computational modeling provides an efficient method for studying the effects of ion irradiation in materials. Modeling complements experiments, by aiding interpretation and often providing insight into the mechanisms and effects of ion–solid interactions. Traditionally, the effect of ion irradiation on solids has been modeled using cascade simulations, which are molecular dynamics (MD) simulations in which one atom is given a high kinetic energy to initiate a radiation cascade event. Such simulations have made enormous contributions to the understanding of fundamental processes, but they suffer from the limitation that the computational time increases dramatically as the simulated ion energy increases. In addition, standard methods do not take into account the effects of excited electrons, which limits their application to radiation events less than a few hundred keV.

As already noted, energy loss by ions in the low energy regime is dominated by nuclear energy dissipation in atomic collision cascades that are readily described by MD methods [22,23], but often without any consideration of the electronic energy losses by primary and secondary ions, which are not completely negligible. For many ionic and covalent compounds, the electronic energy losses in this energy regime can be substantial; thus, MD simulations are beginning to take the electronic energy losses into account as a friction force in order to correctly describe the energy partitioning processes [24,25]. At much higher energies where energy loss to electrons dominates, the relationship between electronic energy loss mechanisms and atomic processes can be described by an inelastic thermal spike model, originally proposed by Vineyard [26] and more fully developed recently [27]. In this model, the electrons along the ion path undergo a large degree of excitation and electron–electron scattering, and they subsequently transfer much of their energy, via electron–phonon coupling, to atoms in the same region, causing local heating. The electronic energy deposition profiles can be determined from either Monte Carlo (MC) methods [28,29] or an empirical expression [30], and energy dissipation within the electronic structure and transfer to the atomic structure is described by a two-temperature model [31]. At intermediate energies where ions transfer substantial and comparable energy to both the electronic and atomic structures, the response of materials is dependent on the complex interaction of electronic excitations, structural atoms and atomic defects. This partitioning of energy deposition, electronic excitation, and energy/heat dissipation are important to both the ion beam modification and radiation damage communities. Under ion irradiation, electronic energy transfer (electronic excitations and electron–phonon coupling) and momentum transfer (atomic collisions) are entangled with equilibrium heating and nonequilibrium excitation processes. To model such complex processes in accurate detail is a grand challenge that demands fundamental

understanding of materials processes at the level of electrons and atoms over several orders of magnitude in time scales, from femtoseconds (fs) to nanoseconds (ns).

2.1. Two-temperature model for ion–solid interactions

While surface modification of materials using ions with energies below a few tens keV can be well modeled by simple cascade simulations, the modeling of ion beam modification processes at the higher energies of interest in this review is less developed. The dominant energy loss process for energies of several MeV/u is inelastic electronic scattering, and this energy loss induces a narrow track of highly excited electrons. These highly excited electrons rapidly distribute their energy through electron–electron interactions (<0.5 ps) until the electrons are sufficiently thermalized to dissipate their energy via electron–phonon coupling to the atoms in the material (0.1–10 ps). It is the dissipation of this energy in a local inelastic thermal spike, followed by a rapid cooling stage (<100 ps), that can result in permanent structural modifications, which can be in the form of damage production, such as defects or an ion track, or the recovery of pre-existing damage. In reality, the dissipation mechanisms are complex and strongly material dependent, but simple models have been developed that capture the dominant features.

The most widely used models are based on the premise that the excited electrons rapidly equilibrate and therefore a temperature, T_e , can be assigned to the electrons. Initially the electrons are far from equilibrium with the atoms, which have a different temperature, T_l [31]. Methods based on this two-temperature approach treat the electronic and atomistic systems as coupled continuous media, whose heat transport properties are governed by two coupled heat diffusion equations. Energy exchange between the electrons and atoms is proportional to the local temperature difference and the electron–phonon coupling constant. The coupled heat diffusion equations for the electronic and ionic temperatures are:

$$C_e \frac{\partial T_e}{\partial t} = \nabla \kappa_e \nabla T_e - g_p (T_e - T_l) + A(\mathbf{r}, t) \quad (1)$$

$$C_l \frac{\partial T_l}{\partial t} = \nabla \kappa_l \nabla T_l + g_p (T_e - T_l) \quad (2)$$

Here C_e and C_l are the electronic and lattice heat capacities, respectively, κ_e and κ_l are the electronic and lattice thermal conductivities, and g_p is the electron–phonon coupling constant. $A(\mathbf{r}, t)$ is the energy deposited to the electronic system as a function of space (\mathbf{r}) and time (t).

The rapid passage of energetic ions through the material allows us to impose radial symmetry around the ion track, and the equations reduce to coupled one dimensional equations that depend only on the radial distance from the center of the ion track. In this case, the source term $A(\mathbf{r}, t)$ is the energy input to the electrons due to inelastic interactions with the swift heavy ion, which can be estimated from Monte Carlo simulations [28,29] or approximated by an analytic function [30]. The time evolution of the spatial distribution of the lattice temperature, or inelastic thermal spike, is determined by numerical solution of the equations. Comparison with experimental observations is made by assuming that the observed track is formed by melting and solidification to an amorphous or highly defective structure. Thus, the spatial extent of the solid that has exceeded the melting temperature corresponds to the calculated track diameter, which can be directly compared with measured tracks.

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