Phonon Production and Nonequilibrium Transport From Ion Strikes

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***Abstract*—Traditionally, prediction of the failure of microelectronic devices due to heavy ion strikes has involved an equilibrium charge production model and subsequent device simulation. However, this approximation has become inadequate for highly scaled devices both in terms of ionizing and nonionizing models. The present work considers nonequilibrium thermal generation and transport resulting from ion strikes, which augments existing models to account for localized heating effects. Using an linear energy transfer model for phonon generation and a Monte Carlo approach to solve for the transport, the nonequilibrium thermal energy distribution is calculated. The resulting energy distribution is correlated to damage cascades, amorphous areas surrounding strike paths and melt regions. Further, the resulting temperature rises can be coupled to device simulations for devices experiencing ion strikes.**

***Index Terms*—Linear energy transfer (LET) model, monte carlo approach, phonon generation.**

I. Introduction

THE interaction of radiation with materials is a complex physical phenomenon that has received considerable attention from both scientific communities and engineers. Electronic devices are particularly interesting to study because the charge produced can result in catastrophic failure. In fact, simulations of the breakdown of devices routinely produce calculations based on a linear energy transfer (LET) and ionization energy [1]. The LET describes the amount of energy deposited into a device per track length and per material density. This energy is then used in conjunction with the well established ionization energy for pair production to obtain the amount of charge created for a given strike. If the spurious charge is large enough to turn on parasitics (in the case of metal oxide semiconductor field effect transistors (MOSFETs) for example), the strike can result in device failure [2].

In many devices, this type of analysis may be adequate to predict the possibility of failure. However, the LET approach in electronic simulations is an average quantity that ignores many physical effects that become significant particularly for highly scaled devices. Examples of higher order effects not normally considered include nonuniform charge generation, secondary ionizing particle creation, nuclear reaction and spallation products, defect generation and cascade damage, nonequilibrium charge production, relativistic particle energies, thermalization, and nonionizing energy loss. Despite the lack of physical rigor, stopping power calculations have proven remarkably successful at generating average track quantities since 1948 when Neils Bohr presented the classical energy loss formula [3]. (The first presentation of this material should be credited to Livingston and Bethe [4].) In highly scaled devices, though, rare events and nonequilibrium effects that deviate from “average” can have significant consequences. This feature, in part, is what has prompted the development of nonionizing energy loss (NIEL) models [5], [6], which attempt to fit measured data for ionization and nuclear reactions. Despite its limitations [7], NIEL can provide a fairly accurate estimate of the thermal component to energy loss for some materials and energy ranges.

Despite recent attention to nonionizing energy losses, device simulation normally considers charge production during a radiation event only. The fact that a portion of the ionization energy appears in the form of phonons is typically ignored. However, Shockley [8] suggests that the majority of the ionization energy goes to the production of phonons. In actuality it can be argued that very little energy of an incident particle is converted directly to lattice vibrations (or phonons). The difference in these two premises is that Shockley assumed that the nonionized energy was already thermalized. As an incident particle interacts with a lattice, energy is lost by the particle as electron/hole pair generation, electron kinetic energy, knock-on atom momentum and Coulomb-generated lattice vibrations. The ratio of lattice vibration energy to the total energy lost by the particle is of the order of 0.1% [3]. However, much of the electron kinetic energy and most of the displacement damage from cascades are thermalized and end up as lattice vibrations [9]. Therefore, Shockley’s estimates can be considered accurate once the the energetic processes have thermalized.

The present analysis considers thermal generation and nonequilibrium transport in semiconductors resulting from an ion strike. While the role of thermal spikes in creating damage has been studied [10], [11], nonequilibrium generation and transport has not rigorously been considered. Conversely, nonequilibrium phonon generation has been considered in photonic excitation experiments [12], but transport was essentially ignored. Interestingly, the photonic excitation experiments in GaAs showed that longitudinal optical excitation dominated the relaxation bottleneck resulting in reduced cooling rates than if equilibrium were assumed. Nevertheless, definitive local temperatures and corresponding melting rates can not be accurately predicted because of the lack of nonequilibrium analysis.

The present simulations follow the approximations provided by Shockley, but the analysis suggests that a more rigorous

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model of phonon production could be useful. In the present context, phonon generation is based on a comparison of mean-free paths between phonon scattering events and ionization events. Details can be found elsewhere [8], but essentially an estimate of the number of phonons produced during an ion strike can be obtained by the ratio of mean free paths. In addition, an energy equivalent to the band gap energy is also committed to phonon production because the band gap represents a threshold below which no pairs can be produced. In the case of silicon, which has an indirect band gap of $E_g \approx 1.1$ eV, the ionization energy is 3.6 eV. Of this quantity, Shockley predicts that $2E_g$ goes into phonon production, 1.1 eV goes into pair production, and the remainder is presumably in the form of electron kinetic energy.

Traditionally, phonon generation and transport from ion strikes has been ignored in device simulation because the effect is secondary if not negligible compared to pair production in devices. The effect can typically be neglected because the phonons are highly localized and do not affect the device performance like spurious charge does. In the case of secondary particle creation, phonon generation can occur away from the primary or initial strike path, but the created phonons are still local to their respective generation region. As energetic particles and electrons transfer energy to lattice vibrations, only the high energy modes (optical phonons) are involved [13], [14]. These high energy modes have negligible group velocity and do not transport significant amounts of energy. Transport occurs only after optical phonons decay or scatter with acoustic phonons that generally transfer energy at the sound speed. By comparing optical phonon lifetimes ($\tau \sim 10$ ps) to electron transport, the localization of thermal energy becomes apparent. This feature is called the "phonon bottleneck" [15, section 1-7-1]. Further, the speed of thermal energy transport (sound speed) is several orders of magnitude smaller than saturation velocities for electrons. Therefore, for reasonably sized devices, the thermal energy does not have a chance to propagate throughout the device before the additional charge has already destroyed the device. In addition, the amount of phonon energy is really quite small compared to the stored thermal energy of devices operating at room temperatures, so the extra energy can be absorbed without affecting the overall condition of the device.

However, the effects of thermal energy in ion strikes becomes significant for highly scaled devices. For example, at a specified LET, the energy deposition rate does not change. Yet as device sizes decrease, the stored energy in the device decreases linearly with the volume. Consequently, the energy deposited as phonons can contain a significant portion of the existing energy in the device, thereby dramatically increasing the device temperature. Implied in this discussion is the confinement of the generation of phonons to the strike radius. Because phonons are generated by Coulomb interactions, the present work assumes that the generation region for phonons corresponds to the strike radius of e-h pair generation. This approach is perhaps not entirely physical but provides a first-order approximation. Additional work is required to understand the size and distribution of phonons within the initial generation region.

Realize that the present discussion does not address thermal energy generated by excessive current (Joule heating). The fact remains that, coupling thermal generation with strike induced current has been shown to play an integral role in device burnout [16]. In the referenced work, compact models for MOSFETs and continuum heat conduction were solved iteratively to predict a secondary breakdown mechanism resulting from ion strikes that can *not* be predicted without the inclusion of thermal effects in simulations. Furthermore, thermal effects have been identified by several researchers as significant contributors to burnout in diodes [17], [18]. Through Joule heating, strike induced charge can result in local temperatures that exceed the melting temperature of silicon [19], [20]. However, none of these simulations consider the nonlocal effects of phonon transport.

In the present work, Monte Carlo simulations predict the nonequilibrium transport of phonons generated in electronic materials along ion tracks. The simulations consider small time and length scales to observe the nonequilibrium propagation of thermal energy in highly scaled devices. The effective temperature rise and time scales for the rise to occur are also estimated. The present work represents an initial investigation into the effects of thermal energy on device performance. Previous work by the authors [20]–[22] has shown that coarse nonequilibrium thermal models can significantly impact the prediction of the thermal response in devices. The purpose of this work is to further demonstrate the importance of thermal effects in ion strike applications and to demonstrate nonequilibrium thermal transport at small scales. The analysis shows that devices of the order of modern CMOS technology are susceptible to thermal effects during ion strikes. Efforts to couple electronic and thermal transport are limited, and this work represents the first attempt to develop models that include phonon dispersion, polarization and multiple scattering mechanisms for electronic simulations of ion strikes.

It is important to place the present analysis into the context of device failure due to radiation. Thermal effects alone will generally not result in failure. However, the thermal effects are coupled to other significant physical phenomena such as electronic properties, energy loss mechanisms and defect development. Fig. 1 provides a skeleton summary of some of the radiation effects that are now being investigated and calculated. The thermalization bubble contains many type of complex models and is difficult to define explicitly. Essentially, the high-energy, nonequilibrium phenomena will relax over a short period of time to an equilibrium or near equilibrium distribution of electrons and phonons. At this point Boltzmann-type solutions (Boltzmann moments with relaxation time approximations) can predict the transport of this simplified system. These techniques are well-established. In addition, significant progress has been made recently on the top portion of Fig. 1. Tools such as GEANT4 and MCNPX can stochastically predict energetic particle trajectories, secondary particle production and energy loss down to a keV. However, little attention has been paid to thermalization. This is where Shockley's model and LET play an important role. They are still the primary techniques for generating charge for device-level simulation. For this reason, we have employed an LET/Shockley approximation when predicting phonon generation. The present analysis, then, represents one piece of the thermalization model.

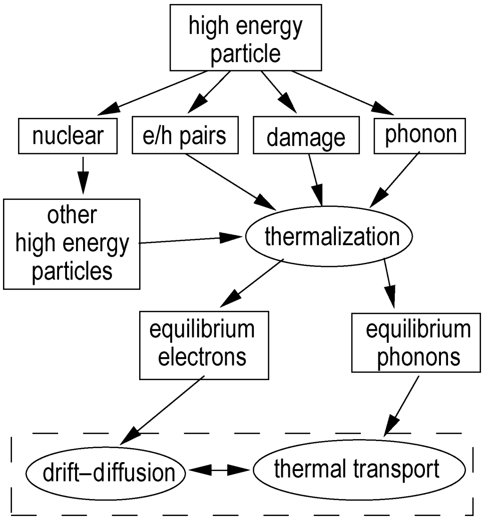

Fig. 1. Schematic representation of the relationship of thermal effects and other physical phenomena that are important to device behavior during radiation events. The dashed box represents the models for typical device simulation.

II. THEORY

The energy deposited as phonons can be calculated similarly to the charge density generated as a result of an ion strike. The total energy deposited during an ion strike is given in terms of its LET

$$E_s = \mathrm{LET}\rho L \tag{1}$$

where L is the track length and ρ is the material density. The ionization energy E_i, which is considered a constant derived by Shockley [8] and verified experimentally for a variety of electronic materials, gives the average energy loss required to create a single electron/hole pair. The number of pairs is then given as E_s/E_i. Using Shockley's approximation for silicon, the energy in phonon production per pair is $E_t' = 2E_g = 2.2$ eV, and the ratio of thermal energy to ionization energy is $E_t'/E_i = 0.61$ (where E_t is thermal energy and the prime indicates per pair).

The production of phonons is presumably a nonequilibrium process. Optical phonons, which have larger frequencies, are excited by Coulomb interactions between the energetic particle and the lattice, electron/hole pair recombination and lattice displacement. Optical phonons, which have negligible group velocity and do not transport energy, will scatter with and decay into acoustic phonons. The relaxation time from optical to acoustic phonons is approximately $\tau = 10$ ps [15]. Therefore, the production of acoustic phonons capable of transporting thermal energy is not an instantaneous process compared to strike dynamics. A Monte Carlo approach can account for this nonequilibrium effect by modeling an ensemble of thermal carriers with different frequencies, polarizations, branches and dispersions.

The thermal energy in a lattice per unit volume can be described in terms of the phonon contribution given as [23]

$$E_l = \sum_p \int_\omega \left(\langle n\rangle + \frac{1}{2}\right)\hbar\omega D(\omega)d\omega \tag{2}$$

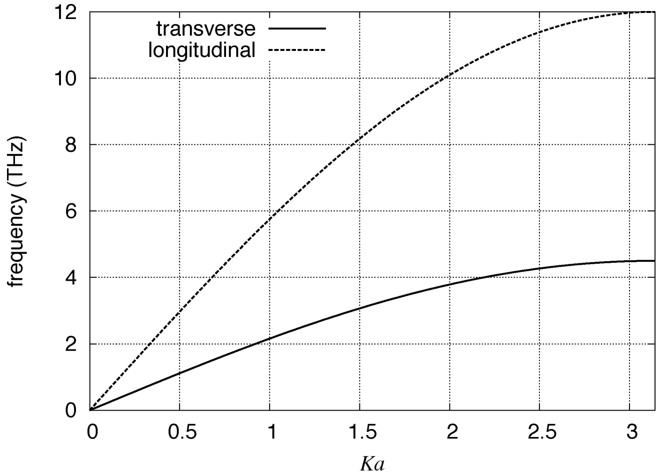

Fig. 2. Analytic dispersion relation for silicon. The slope of the curve is group velocity.

where the energy of a single oscillator is $\hbar\omega$, and the three dimensional density of states per unit volume $D(\omega)$ is expressed as [24, p. 172]

$$D(\omega) = \frac{K^2}{2\pi^2}\frac{dK}{d\omega}. \tag{3}$$

Note that the inverse of the differential is the group velocity determined from the dispersion relation. The excitation number $\langle n\rangle$ is given by the Bose-Einstein distribution

$$\langle n\rangle = \frac{1}{\exp\left[\frac{\hbar\omega}{k_B T}\right] - 1}. \tag{4}$$

The summation in (2) is over all polarizations, which, for the phonon transport, include one longitudinal acoustic branch and two transverse acoustic branches. The dispersion of each branch is shown in Fig. 2, where transverse modes oscillate perpendicular to the direction of motion, and longitudinal modes vibrate in the direction of motion. To obtain the thermal energy in a discretized cell (2) is multiplied by the volume of the cell. Details of phonon properties are found elsewhere (chapters 22 and 23 in [25] or chapter 1 in [26]). For simplicity and computational time, the momentum space is considered isotropic. In general, the dispersion and therefore group velocity is different along different crystal directions. For the present analysis, the differences are small enough not to affect the results significantly. The pre-strike phonon ensemble is chosen randomly from the available branches and polarizations such that the total energy is equivalent to the equilibrium energy at 300 K, and the ratio of the energy from each branch is also the equilibrium ratio [see (2)]. During generation, phonons are created by randomly creating new phonons from the equilibrium distribution until the energy of the lattice calculated by (2) is equal to the thermal energy deposited by the ion strike [(1) scaled by E_t/E_s]. The equilibrium distribution is determined by setting the temperature in (4) to 300 K.

During the Monte Carlo simulation, phonons are allowed to drift (free flight) and scatter. Phonon–phonon scattering includes both normal and Umklapp scattering mechanisms and the scattering rates are given by Holland [27] as frequency and temperature dependent expressions. Details of the Monte Carlo approach can be found elsewhere [23], but essentially phonons are tracked for a small fixed amount of time. At the end of free flight, each phonon in the ensemble is allowed to scatter if random processes allow it. Upon scattering a new momentum and frequency are chosen randomly from the equilibrium distribution. Because the scattering process does not conserve energy, phonons are removed or added to the ensemble to bring the energy back to its level before the scattering process was implemented. In this way, the scattering processes as modeled return the system to equilibirum as in a physical system. Because we are interested in the propagation of energy from the strike, only short times are considered and boundary effects can be effectively ignored.

III. Results and Discussion

Using the LET/Shockley model, bulk quantities can be calculated that give an order of magnitude impact of strike induced thermal energy. Consider a strike in a silicon film that is 100 nm thick (along the direction of the strike) with $\mathrm{LET} = 20\ \mathrm{MeV\ cm^2/mg}$. From (1), the total energy deposited is 4.66×10^5 eV. Because the ionization energy for silicon is 3.6 eV/pair, the number of pairs produced is 1.29×10^5. Because the ratio of thermal energy to strike energy is 0.61, the amount of thermal energy deposited by the strike is 2.84×10^5 eV.

To determine whether this is a significant amount of energy relative to a device, we can calculate the amount of thermal energy in a volume of silicon from (2). For this calculation, we have assumed an isotropic dispersion relation with a maximum frequency of 1.2×10^{13} Hz for the longitudinal branch and 8.6×10^{12} Hz for the transverse branches (see Fig. 2). Fig. 3 shows the equilibrium thermal energy at 300 K for a range of characteristic lengths (side of a cube). For a characteristic length of 100 nm, the thermal energy introduced by the strike is comparable to the equilibrium thermal energy in the device based on a temperature of 300 K. This suggests that small devices are susceptible to thermally induced failure regardless of the charge production by an incident ion.

Also from the total amount of energy deposited, we can approximate the volume of silicon that can be melted by the strike. The melt radius R_m is defined as the maximum distance from the strike that could be melted if all the energy were contained within the melt radius. Therefore, the value follows from the energy required to raise the temperature ΔT and the heat of fusion $\Delta h_f = 1787\ \mathrm{kJ/kg}$, assuming a cylindrical volume about the strike path

$$E_t = 0.61 E_s = \rho \pi R_m^2 L [C \Delta T + \Delta h_f] \qquad (5)$$

where ρ is the material density and $C = 712$ J/kg K is the bulk specific heat. This approximation is shown in Fig. 4 for different LETs in silicon. Realize this analysis does not consider transport away from the strike location, nonequilibrium temperature distribution between phonon modes and microscale effects on material properties. As a result, the bulk approximation over predicts the melt radius but should give an order of magnitude estimate. Note that Williams and Giordano [28] report a melt radius of 70 Å for ^{252}Cf in mica. The properties of mica are similar to silicon and the measured melt radius is about half that predicted by the bulk analysis, which corresponds to our expectations.

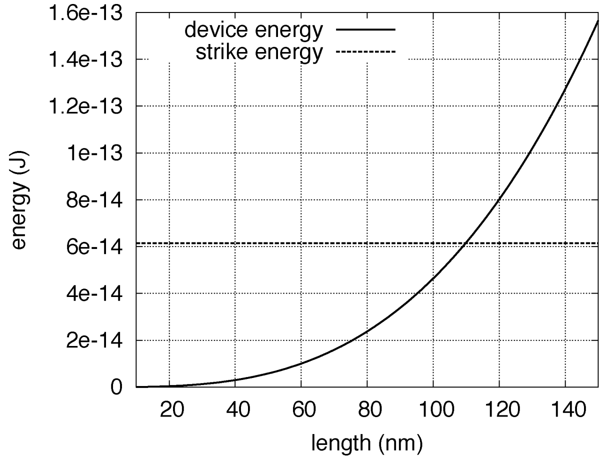

Fig. 3. For devices less than 110 nm on a side (volume of 10^{-21} cm^3), an ion with an LET of 20 MeV cm^2/mg will produce more thermal energy than exists in the device. Energy deposited by the strike increases linearly as the dimension along the strike direction. However, intrinsic thermal energy increases as the cube of the dimension of the device.

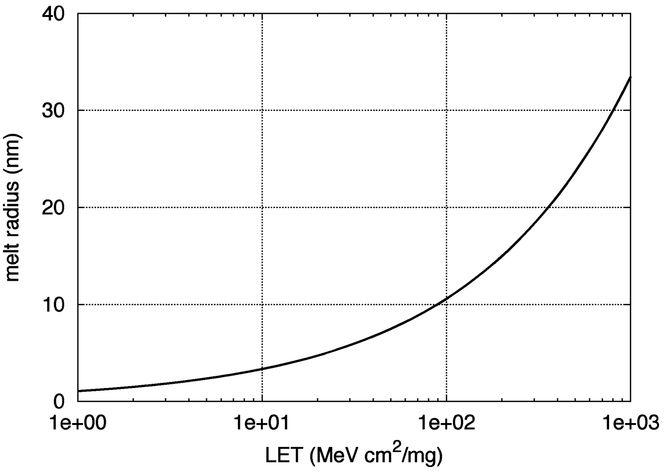

Fig. 4. Bulk approximation to melt radius [R_m in (5)] over predicts the actual melt radius due to microscale effects.

Nonequilibrium and microscale effects are considered in the Monte Carlo phonon analysis. As the phonon energy propagates through the lattice, it will leave a region that experiences extreme temperatures. Because the transport is nonequilibrium in nature, calculated temperatures are not necessarily representative of measured temperatures. Nevertheless, a pseudo temperature can be calculated from the predicted energy by inverting (2) for the temperature in (4). Simulations show that the the melt radius when nonequilibrium transport is considered is roughly half that of the bulk approximation. Even with nonequilibrium analysis, melting is not formally included in the model, so transport within the melt region is suspect. Nevertheless, the prediction matches well with expectations.

The energy travels through the lattice in a wave with a wave velocity that is related to the average group velocity of phonons. The calculated group velocity matches well with known sound speeds for silicon. However, this is little more than a sanity

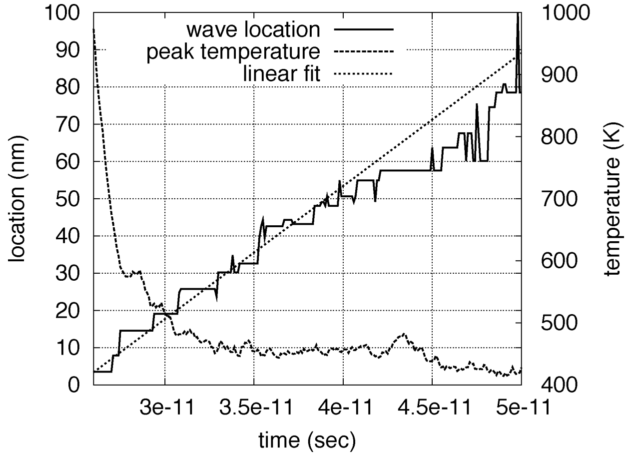

Fig. 5. Results of the Monte Carlo simulation show that the strike creates a wave of nonequilibrium phonon transport that propagates through the device. The slope of the location curve (linear fit) is the average velocity of the wave ($\sim$ 3500 m/s). Notice that the wave dissipates around 4.2×10^{-11} s and that the device temperature has risen to 420 K (on average) from 300 K. The noise is a function of the spatial discretization.

check because the slope of the analytic dispersion relation determines the group velocity. The temperature at the peak of the wave will decrease with distance from the strike because the energy is spread over a larger area. Further, the wave will dissipate as Umklapp scattering processes resist the phonon transport. Fig. 5 shows the radial distance of the wave from the strike location as a function of time and the maximum temperature of the wave. The original device temperature was 300 K, and the average temperature after the wave traverses the device has risen to 420 K. (The peak value from Fig. 5 is 450 K.) At this elevated temperature, device performance can be severely altered. In fact, this value is far above the recommended maximum allowable temperature for many commercial CMOS devices. Therefore, this device is a candidate for failure. For example, the intrinsic carrier concentration at 420 K is 400 times greater than at 300 K [29, Fig. 11, p. 19]. In the depletion region of a MOSFET, this could relate to a significant difference in performance. Another effect of elevated temperature is decreased mobility due to increased phonon scattering. A temperature rise from 300 K to 420 K represents a 10% decrease in the saturation velocity [30], which also suggests a definite change in performance.

The resident time of the energy near the strike location is important because it affects rapid annealing and defect migration. In the simulations, most of the energy stayed within 5 nm of the strike path for 20 ps, and a large portion of the energy remained for 50–100 ps. This is the region where most of the cascade damage occurs [31]. Note that most cascade events occur within 10 ps, so a large amount of thermal energy is available to assist in defect reorganization. In fact, molecular dynamics studies have confirmed that most cascade regions are reduced to a few Frenkel pairs in tens of picoseconds [32]. Likewise, measurements of damaged regions have shown that damage and recovery occurs within a $\sim$ 10 nm diameter area [33].

Although ion implantation for doping is not an operational issue for semiconductor devices, the present analysis can be used to make predictions on the efficacy of processing parameters because the thermal interactions are similar. For highly scaled devices, the accurate knowledge about the density and range of implantations becomes increasingly important and difficult to know [34]. In fact, Peltola and Nordlund [35] found that the depth of ion implantation is significantly less for amorphous materials than for crystalline materials. If ion implantation causes enough local heating to induce melting, then the depth of subsequent implantations would be reduced, and the doping density could be different than originally expected.

IV. CONCLUSION

In general, nonequilibrium thermal effects associated with ion strikes have been ignored because the thermal energy production is small relative to the intrinsic energy based on a device's temperature. However, the present work shows that the thermal energy production may be significant enough to affect highly scaled devices. In fact the total energy of a 90 nm technology can see a doubling of its intrinsic energy as a result of a 20 MeV cm^2/mg LET strike. Simulations of the energy propagation also demonstrate that nonequilibrium transport has significant effect on annealing and possibly device performance. This paper provides the impetus for further investigation into nonequilibrium thermal generation and transport resulting from ion strikes. In addition, the integration of nonequilibrium thermal models with electron transport models is crucial to predicting device performance.

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