PHONON PRODUCTION, NONEQUILIBRIUM TRANSPORT AND EFFECTS FROM ION STRIKES

D. G. Walker and R. A. Weller

Vanderbilt University, Nashville, TN

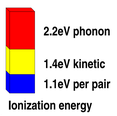
A portion of the energy transmitted to the lattice by an incident particle could reappear in the form of lattice vibrations in so concentrated a way that the local temperature would be sufficiently high to induce permanent rearrangement of the atoms of the solid. ***– Seitz and Koehler (1956)***

Thermal Physics Laboratory

Department of Mechanical Engineering
Department of Electrical Engineering
Radiation Effects and Reliability Group
Vanderbilt University Discovery Grant

Summary

- Ionizing radiation in materials creates electron/hole pairs and phonons [1]
- Partitioning of phonon energy to electronic energy is comparable
- Phonon transport is characterized by non−equilibrium at small scales commensurate with todays nanometer devices
- **Localized phonon production and transport (heating) from single ionizing events can be significant**

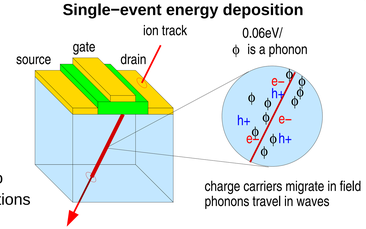


[1] W. Shockley, "Problems related to $p-n$ junctions in silicon," *Solid-State Electronics*, **2**(1), pp. 35–60, 1961.

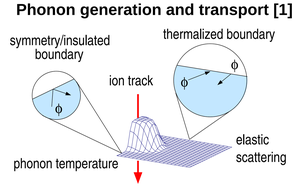
Model

- Linear energy transfer (LET) is used here to predict number of phonons generated during an ion strike.
- Phonons travel in waves, scatter and result in localized high temperatures.
- Monte Carlo approach is used to solve Boltzmann transport equations with full dispersion.

Single−event energy deposition



Phonon generation and transport [1]



Phonon number	$N = \sum_p \sum_{i=1}^{N_b} \langle n(\omega_i)\rangle D(\omega_i)\Delta\omega_i$
Occupation	$\langle n\rangle = \left[\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1\right]^{-1}$
Temperature	$\frac{E}{V} = \sum_p \sum_{i=1}^{N_b} \frac{\hbar\omega_i D(\omega_i)\Delta\omega_i}{\exp\left(\hbar\omega/k_B T\right) - 1}$

- $D(\omega)$ is the density of states, which is dependent on the dimensionality.
- $\sum_p$ is the summation over polarizations and phonon branches (transverse vs. longitudinal and acoustic vs. optical).
- The frequency is discretized, and N_b is the number of intervals.
- V is volume of an element in the discretized spatial domain.

Time scales
strike time
relaxation time
decay time

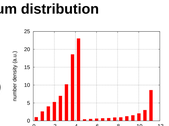
Length scales
device size
phonon mean free path

Velocities
wave velocity
group velocity

- Characteristic lengths and times are related through characteristic velocities.
- Thermalized boundaries absorb incident phonons and reemit equilibrium phonons.
- Insulated boundaries reflect perfectly.

Equilibrium distribution

Transverse acoustic branch (lower frequency) dominates



Scattering types and rates [2]

Impurity scattering

$$\tau_i^{-1} = \alpha\sigma\rho|\mathbf{V}_g|, \quad \mathbf{V}_g\text{:group velocity}$$

$$\sigma = \pi r^2\left(\frac{\chi^4}{\chi^4+1}\right), \quad \chi = r|\mathbf{K}|$$

3–phonon processes

Normal: conserve energy and momentum

$$\tau_{NU}^{-1} = B_L\omega^2 T^3$$
$$\tau_N^{-1} = B_{TN}\omega T^4$$

Umklapp: conserve energy but not momentum

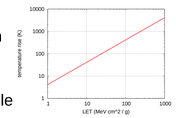
$$\tau_U^{-1} = \begin{cases} 0 & \omega < \omega_{1/2} \\ B_{TU}\omega^2/\sinh\left(\frac{\hbar\omega}{k_B T}\right) & \omega > \omega_{1/2} \end{cases}$$

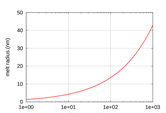
[1] S. Mazumder and A. Majumdar, "Monte Carlo study of Phonon transport in solid thin films including dispersion and polarization," *Journal of Heat Transfer*, **123**, pp. 749–759, 2001.
[2] M.G. Holland, "Analysis of lattice thermal conductivity," *Physical Review*, **132**(6), pp. 2461–2471, 1963.

Simulation Results

Bulk Approximation

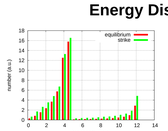
For a small SOI device (100nm x 100nm x 100nm), an ion will deposit enough energy to result in a significant temperature rise, suggesting damage is possible





The "melt" radius corresponds to the damage profile predicted by cascades [1]. However, this estimate does not account for heat removal by the surrounding material.

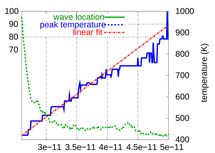
Energy Distribution



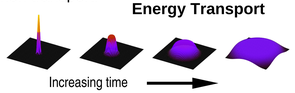
The distribution of phonons after the strike is shifted toward high−energy modes (longitudinal acoustic), which shows nonequilibrium distribution is averaged over entire domain at 25 picoseconds

Nonequilibrium Analysis

Energy travels in the lattice as a wave. Wave velocity is related to group velocity of phonons (2200 m/s in bulk). Temperature at the wavefront will decrease as the wave travels because energy is distributed over a larger volume. Further the wave will dissipate as Umklapp scattering resists phonon transport.



Energy Transport



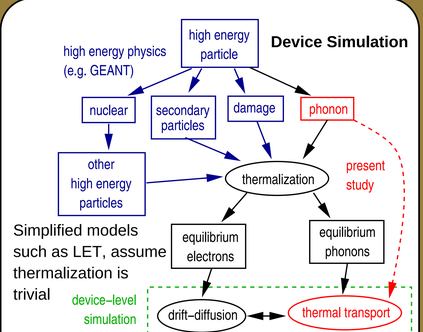
[1] T. Díaz de la Rubia, "Irradiation-induced defect Production in elemental metals and semiconductors: A review of recent molecular dynamics studies," *Annual Reviews of Materials Science*, **26**, pp. 613–649, 1996.

Conclusions

- The foregoing demonstration illustrates the exigency of including thermal effects in single-event radiation-induced failure of highly scaled devices.
- Localized temperatures can exceed thousands of degrees (realize that temperature is only formally defined in equilibrium [2], which does not exist in this case).
- Displacement cascade damage can be interpreted as a nonequilibrium thermal spike [1] where localized melting and reconstitution occur uniformly about the ion track.
- The present analysis is but one piece of a bigger picture. Phonon generation (from GEANT4- or SRIM-type simulations) and device-level simulation are the bookends for the present analysis.

[1] T. Diaz de la Rubia, R.S. Averback, R. Benedek, W.E. King, "Role of thermal spikes in energetic displacement cascades," *Physical Review Letters*, **59**(17), pp. 1930–1933, 1987.
[2] D.G. Cahill, W.K. Ford, K.E. Goodson, G.D. Mahan, A. Majumdar, H.J. Maris, R. Merlin, S.R. Phillpot, "Nanoscale thermal transport," *Journal of Applied Physics*, **93**(2), pp. 793–817, 2003.

Context



Simplified models such as LET, assume thermalization is trivial

Rigorous nonionizing energy loss [1] can now be calculated and used as initial conditions for phonons

[3] R.A. Weller, M.H. Mendenhall and D.M. Fleetwood, "A screened Coulomb scattering module for displacement damage computation in GEANT4," *NSREC poster* #ph4, 2004 **Please see!**.

Applications/Impact

Manufacturing Nanowires

Radiation-induced melting is used to create channels for nanowire production [1]. Bulk analysis over predicts bulk approximation of melt radius because transport away from the strike is not considered and nonequilibrium temperatures can not be clearly defined.

Energy Available for Rapid Annealing

Presence of localized thermal energy can accelerate defect reordering [2]. Presumably different amounts of thermal energy are deposited by different ions even for similar particle energies. Therefore, some ions produce less defects because more thermal energy is available for rapid annealing. Note that NIEL does not predict the division of pure thermal energy (phonons) and displacement damage, so by itself, NIEL can not predict the eventual defect distribution.

Thermal Spikes/Melting and Displacement Damage

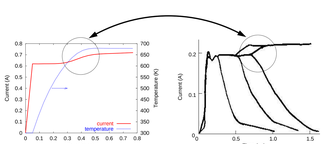
- Thermal spikes and local melting affect defect production and cascade damage development.
- Diffusion analysis [3] does not account for nonequilibrium temperatures.
- Molecular dynamics [4] can not model wave-like nature at boundaries.

Ion Implantation

Ion implantation produces thermal energy, which in turn affects the scattering cross section of the lattice. Ion implanted at a latter time will not penetrate as far due to thermal effects.

Device Transients

Temperature is intimately linked to device performance. Only with a model the includes thermal transport can the secondary increase in current that is observed be predicted [5].



[1] W.D. Williams and N. Giordano, "Fabrication of 80Å metal wires," *Rev. Sci. Instrum.*, **55**,(3), pp. 410–412, 1984.
[2] J.R. Srour, C.J. Marshall and P.W. Marshall, "Review of displacement damage effects in silicon devices," *IEEE Trans. Nuclear Sci.*, **50**(3), pp. 653-670, 2003.
[3] F. Seitz and J.S. Koehler, *Displacement of Atoms During Irradiation*, in Solid State Physics, Vol. 2, eds. F. Seitz and D.Turnbull, 1956.
[4] T.D. de la Rubia, R.S. Averback, R. Benedek and W.E. King, "Role of thermal spikes in energetic displacement cascades," *Phys. Rev. B*, **59**(17), pp. 1930–1933, 1987.
[5] D.G. Walker, T.S. Fisher, J. Liu and R.D. Schrimpf, "Thermal Modeling of Single Event Burnout Failure in Semiconductor Power Devices," *Journal of Microelectronics Reliability*, **41**(4), pp. 571-578, 2001.

Future Work

- Use high-fidelity particle tracking simulations as initial conditions for phonon transport
- Couple thermal response to electrical behavior (device simulation) and damage models (molecular dynamics boundary conditions).