Designation: E3084 – 17

Standard Practice for Characterizing Particle Irradiations of Materials in Terms of Non-Ionizing Energy Loss (NIEL)[1]

This standard is issued under the fixed designation E3084; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This practice describes a procedure for characterizing particle irradiations of materials in terms of non-ionizing energy loss (NIEL). NIEL is used in published literature to characterize both charged and neutral particle irradiations.

1.2 Although the methods described in this practice apply to any particles and target materials for which displacement cross sections are known (see Practice E521), this practice is intended for use in irradiations in which observed damage effects may be correlated with atomic displacements. This is true of some, but not all, radiation effects in electronic and photonic materials.

1.3 Procedures analogous to this one are used for calculation of displacements per atom (dpa) in charged particle irradiations (see Practice E521) or neutron irradiations (see Practice E693).

1.4 Guidance on calculation of dpa from NIEL is provided.

1.5 Procedures related to this one are used for calculation of 1-MeV equivalent neutron fluence in electronic materials (see Practice E722), but in that practice the concept of damage efficiency, based on correlation of observed damage effects, is included.

1.6 Guidance on conversion of NIEL in silicon to monoenergetic neutron fluence in silicon (see Practice E722), and vice versa, is provided.

1.7 The application of this standard requires knowledge of the particle fluence and energy distribution of particles whose interaction leads to displacement damage.

1.8 The correlation of radiation effects data is beyond the scope of this standard. A comprehensive review (**1**)[2] of displacement damage effects in silicon and their correlation with NIEL provides appropriate guidance that is applicable to semiconductor materials and electronic devices.

2. Referenced Documents

2.1 *ASTM Standards*[3]

E170 Terminology Relating to Radiation Measurements and Dosimetry

E521 Practice for Investigating the Effects of Neutron Radiation Damage Using Charged-Particle Irradiation

E693 Practice for Characterizing Neutron Exposures in Iron and Low Alloy Steels in Terms of Displacements Per Atom (DPA), E 706(ID)

E722 Practice for Characterizing Neutron Fluence Spectra in Terms of an Equivalent Monoenergetic Neutron Fluence for Radiation-Hardness Testing of Electronics

3. Terminology

3.1 Definitions of some terms used in this practice can be found in Terminology E170.

3.2 *Definitions:*

3.2.1 *tracked particles*—those particles whose position-dependent fluence spectra are calculated in a particle transport calculation for a specific target geometry.

3.2.1.1 *Discussion*—In calculating displacement damage energy and NIEL, the tracked particles should include neutrons, photons, protons and ions up to Z=2, unless their contributions are known to be negligible. Heavier ions may also be tracked in some Monte Carlo codes. Except in the case of neutrons, particles below a specified minimum energy are not tracked, and are treated as *non-tracked particles*.

3.2.2 *tracked-particle fluence spectrum,* $\Phi_p(E)$—the fluence spectrum of particles, of species p and at particle energy E, that are tracked in a particle transport calculation. For each species of tracked particle other than neutrons there is a specified minimum energy. Particles at lower energy are non-tracked particles.

3.2.3 *secondary particles*—those particles produced in a material by interaction with the tracked particles. Secondary particles may include tracked particles and non-tracked particles.

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[1] This test method is under the jurisdiction of ASTM Committee E10 on Nuclear Technology and Applications and is the direct responsibility of Subcommittee E10.07 on Radiation Dosimetry for Radiation Effects on Materials and Devices.

Current edition approved Feb. 1, 2017. Published March 2017. DOI: 10.1520/D3084-17.

[2] The boldface numbers in parentheses refer to a list of references at the end of this standard.

[3] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

3.2.4 *non-ionizing energy loss, $NIEL_p(E)$*—the quotient of $d\bar{\varepsilon}_d$ by $\Phi_p(E).dE.dm$, where $\Phi_p(E)dE$ is the tracked-particle fluence in the energy interval E to $E+dE$ of particle species p in a volume element containing material of mass dm, and $d\bar{\varepsilon}_d$ is that part of the mean energy imparted to matter by the tracked particle radiation which produces atomic displacements and lattice phonons (that is, excluding the part that produces ionization and excitations of electrons).

$$NIEL_p(E) = d\bar{\varepsilon}_d / \Phi_p(E)dEdm \tag{1}$$

Unit: MeV·m^2·kg^{-1}. (also used are keV·cm^2·g^{-1}, and MeV·cm^2·g^{-1})

3.2.4.1 *Discussion*—For silicon, using the atomic mass 28.086 g/mol, a displacement kerma cross section 100 MeV·mbarn is equivalent to 2.144 MeV·cm^2/g (**2**). Microscopic displacement kerma cross sections (See Practice E722) having units with dimensions equal to the product of energy and area (for example, MeV·mbarn) are sometimes used, to apply to single target atoms, and may be thought of as the microscopic version of NIEL. For 1-MeV neutrons the reference value of the displacement damage function in silicon is defined in Practice E722 as equal to 95 MeV·mbarn, equivalent to a NIEL value of 2.037 MeV·cm^2/g (0.2037 Mev·m^2·kg^{-1}).

3.2.4.2 *Discussion*—In Eq 1, $NIEL_p(E)$ is to be interpreted as a function dependent on the particle energy, on the species of particle, and on the material in which the particle fluence is present. Its use requires knowledge of NIEL for all energies and tracked-particle species that contribute significantly to the total displacement damage energy in a given material.

3.2.4.3 *Discussion*—In the definition, Eq 1, the volume element in which the tracked-particle fluence Φ_p is present does not necessarily contain all of the atomic displacements produced by the energy transferred, $d\bar{\varepsilon}_d$. The quantity is calculated *as if* the extended volume, dependent on the particle energy, in which displacements occur is homogeneous and of the same composition as the volume element in which the tracked-particle fluence is present. This assumption is justified in cases in which secondary particle equilibrium applies for the non-tracked particles: the number and energy distribution of secondary particles entering a volume element is the same as for those leaving that element. See the analogous description of "charged particle equilibrium" in the definition of **kerma**, E170.

3.2.4.4 *Discussion*—Damage energy per unit mass, $d\bar{\varepsilon}_d / dm$ is calculated from NIEL by integrating the product of the NIEL with the tracked-particle fluence spectrum over all energies, and summing over all species of tracked particle:

$$d\bar{\varepsilon}_d / dm = \sum_p \int_0^\infty NIEL_p(E)\Phi_p(E)dE \tag{2}$$

3.2.4.5 *Discussion*—The 1 MeV equivalent neutron fluence (cm^{-2}) in silicon may be calculated by dividing the damage energy per unit mass (MeV/g) in Eq 2 by 2.037 MeV cm^2/g (see 3.2.4.1).

3.2.4.6 *Discussion*—The dpa may be calculated from the damage energy per unit mass by multiplying by the average atomic mass of the target and by $\beta/2T_d$, where β is an atomic scattering correction factor equal to 0.8 and T_d is the displacement threshold. This approximation to the Norgett, Robinson and Torrens (**3**) model is consistent with the method recommended in Practice E521 (14.5.2.1).

3.2.4.7 *Discussion*—In cases where secondary particle equilibrium does not apply, due to inhomogeneities in the target material, the damage energy that can be calculated from NIEL values is not necessarily equivalent to the local value of the absorbed dose that leads to displacements. The scale of the relevant inhomogeneities depends on the energies and actual ranges of the non-tracked secondary particles. Detailed Monte Carlo modeling in which tracked particles include all those secondary particles whose range is comparable with or greater than the scale of the material inhomogeneity in the target geometry is necessary. Suitable codes include MCNP6, Geant, and SRIM (**4-9**).

4. Significance and Use

4.1 A radiation-hardness assurance program requires a methodology for relating radiation induced changes in materials exposed to a variety of particle species over a wide range of energies, including those encountered in spacecraft and in terrestrial environments as well as those produced by particle accelerators and nuclear fission and fusion reactors.

4.2 A major source of radiation damage in electronic and photonic devices and materials is the displacement of atoms from their normal lattice site. An appropriate exposure parameter for such damage is the damage energy calculated from NIEL by means of Eq 2. Other analogous measures, which may be used to characterize the irradiation history that is relevant to displacement damage, are damage energy per atom or per unit mass (**displacement kerma**, when the primary particles are neutral), and **displacements per atom (dpa)**. See Terminology E170 for definitions of those quantities.

4.3 Each of the quantities mentioned in the previous paragraph should convey similar information, but in a different format. In each case the value of the derived exposure parameter depends on approximate nuclear, atomic, and lattice models, an on measured or calculated cross sections. If consistent comparisons are to be made of irradiation effects caused by different particle species and energies, it is essential that these approximations be consistently applied.

4.4 No correspondence should be assumed to exist between damage energy as calculated from NIEL and a particular change in a material property or device parameter. Instead, the damage energy should be used as a parameter which describes the exposure. It may be a useful correlation variate, even when different particle species and energies are included. NIEL should not be reported as a measure of damage, however, unless its correlation with a particular damage modality has been demonstrated in that material or device.

4.5 NIEL is a construct that depends on a model of the particle interaction processes in a material, as well as the cross section for each type of interaction. It is essential, when using NIEL as a correlation parameter, to ensure that consistent modeling parameters and nuclear data are used to calculate the NIEL value for each irradiation.

4.6 Damage energy deposited in materials can be calculated directly, without the use of NIEL, using the Monte Carlo codes mentioned in 3.2.4.7, if all the particles involved in atomic displacement are tracked. The utility of the NIEL concept arises in cases where some particles, especially recoiling heavy ions, do not need to be tracked. In the NIEL representation, these are treated instead by means of infinite homogeneous medium solutions of the type originated by Lindhard et al. (**10**).

5. Calcucation of NIEL

5.1 The method of calculating NIEL used in this practice is based on that originally proposed for proton irradiation of silicon by Burke (**11**). Similar NIEL calculations and comparisons to experiment have since been done for other particles and other targets (**12-17**).

5.2 The basic formula for the calculation of NIEL is:

$$NIEL_{\mathrm{p}}(E) = \sum_i N_i \sum_k \int_0^\infty T_k \frac{d\sigma_{\mathrm{p}ik}(E\ ,\ T_k)}{dT_k} L(T_k)\, dT_k \tag{3}$$

where:

$N_i = w_i N_{av}/A_i$ = the number of target atoms of isotope i per unit mass,

w_i = the weight fraction of isotope i in the target,

N_{Av} = is Avogadro's number/mole,

A_i = the molar mass for isotope i,

T_k = the energy of a non-tracked secondary particle, k,

$d\sigma_{\mathrm{p}ik}(E,T_k)/dT_k$ = the differential cross section for collisions of tracked particle, p, in isotope i through all reaction channels resulting in production of non-tracked secondary particle, k, of energy T_k .

$L(T_k)$ = the Lindhard partition function (**10**) describing the fraction of the energy of secondary particle, k, that results in atomic displacements and phonons. The form of the function $L(T_k)$ depends on the species of particle, p, and on the target material.

NOTE 1—Published NIEL calculations have often used T_d as the lower limit of the integral in Eq 3, where T_d is the displacement threshold energy (defined in Terminology E170). It is not used here because damage energy below the displacement threshold contributes to phonons and is non-ionizing. This also maintains consistency with other ASTM standards (E521 and E722). The inclusion of T_d in the calculation has negligible effect in cases of practical interest for irradiation effects in electronic devices.

5.3 Most authors who have used formulae analogous to Eq 3 have followed the precedent of Burke (**11**), but excluding light ions with masses up to and including He-4 from the secondary particles that contribute to NIEL. This is equivalent to treating such particles as tracked particles whose contributions to displacement were ignored.

5.4 Radiation induced damage to the lattice of solid materials arises from elastic collisions and nuclear reactions resulting in high energy recoils. These cause ionization and excitation of the atoms in the irradiated material as well as elastic and inelastic scattering which produce displacement of the atoms from their sites in the lattice. Ionization is a transient effect in many semiconductors and does not contribute to permanent damage in, for example, bulk silicon (**2**). Elastic collisions and inlastic reactions can generate permanent stable lattice defects via what are called displacement cascades. Cascade dynamics are best described by molecular dynamics simulations (**18**) although energy partitioning can also be obtained from Monte Carlo simulations (**4-9**) and other transport calculations.

5.5 The partition of the secondary particle energy T_k between electronic excitation and atomic displacements is reflected in the partition function $L(T_k)$, sometimes called the damage efficiency. Various approximations to the partition function have been used, based on the Lindhard screened potential scattering theory (LSS) (**10**), using the Thomas-Fermi model. An approximation based on the LSS model is given by the Robinson fit (**19**), used also in the NRT model (**3**) for calculating dpa:

$$L(T_k) = \frac{1}{1 + F_L(3.4008\ \varepsilon^{1/6} + 0.40244\ \varepsilon^{3/4} + \varepsilon)} \tag{4}$$

where $\varepsilon = \frac{T_k}{E_L}$, with

$$E_L = 30.724\ Z_k Z_L (Z_k^{2/3} + Z_L^{2/3})^{1/2} (A_k + A_L)/A_L \text{ ,and} \tag{5}$$

$$F_L \frac{0.0793 Z_k^{2/3} Z_L^{1/2} (A_k + A_L)^{3/2}}{(Z_k^{2/3} + Z_L^{2/3})^{3/4} A_k^{3/2} A_L^{1/2}} \tag{6}$$

A and *Z* are mass numbers and atomic numbers and the subscripts *L* and *k* stand for lattice atom and recoil particle, respectively.

5.6 The formula for the partition function given in 5.5 is consistent with that used in Practices E521, E693, and E722. It was also used by Jun (**20**), and by other authors, for NIEL calculations.

5.7 Partition functions other than the NRT fit have been used by some authors, (**21**), and may be preferred in cases when they can be consistently used for all particles and energies.

5.8 Approximations in the original Lindhard model (**10**) and specifically in the Norgett, Robinson and Torrens (NRT) fit (**3**), required that recoil energies, T_k, be limited to less than about $24.8Z^{4/3}A$ (in keV) where *A* is the atomic mass of the lattice atoms and *Z* is the atomic number of the lattice. In iron this limitation translates to a maximum permissible recoil energy of 107 MeV. In silicon, the limitation translates to a maximum permissible recoil energy of 23 MeV.

5.9 The Norgett, Robinson and Torrens (NRT) fit to the LSS theory (**3**) is applicable only in cases where the recoil atom is close in atomic number and atomic weight to the lattice atoms. For this reason the non-tracked secondary particles, designated by subscript *k* in Eq 3, should not include nucleons or light ions when the NRT formulation is used.

5.10 Secondary particles other than non-tracked particles, whether produced in the target material or in its surroundings, may contribute to the total damage energy. If so, they must be treated as part of the local particle fluence spectrum, after calculation of their energy dependent fluence in an appropriate radiation transport code that models the environmental geometry. This applies especially to secondary hadrons (neutrons, protons and mesons) and photons, whose range may greatly exceed typical device dimensions.

5.11 Versatile methods for calculating NIEL have been developed (**13, 14, 15, 20, 22**), and results have been tabulated for a wide range of incident particles (including ions), energies and materials.

5.11.1 Results reported in the references cited in 5.11 were obtained using the damage energy tally in MCNPX (**4**) to score the damage energy in a think target approximation (**20**). In the limit of infinitely thin targets, the energy deposited by particles tracked in MCNPX will not be included in such a score but the energy deposited by non-tracked particles is deposited locally at the point of their production and therefore is included. The versions of MCNPX available at the time these calculations were done included ions of mass up to ^{4}He as particles that could be tracked, but heavier particles were non-tracked. Assuming default options for tracking were used, therefore, it can be inferred that the calculations are equivalent to those described by Eq 3 when all particles of mass up to ^{4}He are tracked, and heavier particles are non-tracked.

5.11.2 Jun et al. (**13, 14, 15, 20, 22**), use the Zieglier-Biersach-Littmark (ZBL) potential (**23**) for screened Coulomb scattering calculations at lower ion energies (less than 50 MeV per nucleon) and Mott-Rutherford calculations at higher energies.

5.11.3 For ion energies per nucleon between 50 MeV and 1000 MeV, the Mott-Rutherford differential cross sections were used for $d\sigma/dT$ (**24**).

5.11.4 The nuclear elastic and inelastic interactions due to protons and alpha particles were accounted for (**13, 14**) by utilizing MCNPX (**4**) and appropriate physics models implemented in the code. If elastic, MCNPX computes the primary knock-on (PKA) energy using standard kinematics. In the case of a nonelastic reaction, MCNPX goes to the high-energy intra-nuclear cascade (INC), pre-equilibrium, and evaporation physics to compute the PKA energy, T, and its final mass and charge.

5.11.5 For incident heavy ions, fragmentation of both the incident ion and the target have to be considered (**22**) at high energies. In such cases, the designation PKA, used in Eq 2 becomes unclear. However, it was found in numerical examples that the contribution of the incident ion fragmentation process to the total NIEL is negligible (**22**).

5.12 Values for NIEL, based on methods similar to those of Jun et al. (**13, 14, 15, 20, 22**) are provided in a web-calculator provided by the AMS-02 Milano Bicocca Group (**25**).

5.13 NIEL values for compounds of elements of similar mass may be derived from the elemental results by weighting the target elemental NIEL value by their weight fractions in the compound. Thus, for gallium arsenide, GaAs, the NIEL value is found by multiplying the gallium value by 69.723/144.645, the arsenic value by 74.922/144.645, and adding the two results.

5.14 Ref (**13**) claims that the method described in 5.13 can be used for compounds of elements with widely different masses. This method of calculation (sometimes called the 'Bragg rule') is not valid, however, when the masses of the constituent elements are very dissimilar (**26-32**). Luneville et al. (**33**) have described a method of calculation by means of the binary collision approximation (BC) that does correctly address the damage energy in polyatomic materials. This method is implemented in the DART code (**34**). "To calculate the number of displacements the DART code does not use the classical NRT dpa analytical formula, which is only appropriate for projectile and target of the same mass. It numerically solves the linearized Boltzmann equation for a polyatomic target."

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