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Behavioral modeling of SRIM tables for numerical simulation

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ABSTRACT

This work describes a simple way to implement SRIM stopping power and range tabulated data in the form of fast and continuous numerical functions for intensive simulation. We provide here the methodology of this behavioral modeling as well as the details of the implementation and some numerical examples for ions in silicon target. Developed functions have been successfully tested and used for the simulation of soft errors in microelectronics circuits.

1. Introduction

Stopping and Range of Ions in Matter or SRIM is a collection of software packages developed by Ziegler and Biersack [1–3] that calculate the stopping and range of ions into matter. SRIM is a reference and extremely popular program in the radiation effects community; it is based on a Monte Carlo simulation method, namely the binary collision approximation with a random selection of the impact parameter of the next colliding ion. Among all functionalities of the developed packages, SRIM includes quick calculations that produce tables of stopping powers, range and straggling distributions for any ion at any energy (in the range 10 eV–2 GeV) and in any elemental target. More elaborate calculations include targets with complex multi-layer configurations [1].

SRIM tables of stopping power, linear energy transfer (LET) and projected range (R) versus particle energy are very useful for the computation of particle transport in a wide range of simulation applications which do not directly involve a specific ion transport code. Although a special independent executable program (SRIM Module.exe) can be used as a subroutine for Windows applications, for other operating systems or simulation frameworks, libraries of fast table lookup and interpolation algorithms are generally necessary to embed SRIM data in the simulation flow. Another alternative, described here, is to use very accurate fitting functions that can be parameterized as a function of the ion parameters, i.e. the atomic number, mass (amu), and kinetic energy. In the following, we detail how SRIM tabulated data can be described in the form of fast and continuous numerical functions. The approach is particularly well adapted for intensive simulation that requires very frequent LET and R calculations for a wide variety of ions, for example for the simulation of single-event effects in microelectronics circuits. We illustrate in the following the details of the implementation of the proposed solution in such a particular application framework.

2. Numerical model and approach

The behavioral modeling of SRIM data has been performed on the basis of power polynomial fitting functions as a function of particle energy (E) for a given ion, a given target and a given energy range. This later has been arbitrarily fixed to a relatively wide interval [1 keV, 1 GeV] that should be suitable for many applications. But nothing prevents a user to choose another energy interval more adapted to its application. After exploring and evaluating a large collection of fitting functions, we definitively adopt the following expressions for modeling the linear energy transfer given by SRIM tables in the defined energy range:

$$\mathrm{LET}(E) = 10^{A(E)} \tag{1}$$

$$A(E) = \sum_{i=1}^{8} a_i \times \sin(b_i \cdot \log_{10}(E) + c_i) \tag{2}$$

where a_i, b_i and c_i correspond to a set of $8 \times 3 = 24$ real coefficients characteristics of a given ion for a given target material.

Similarly, for the projected range versus energy in the same energy domain, we adopt the following modeling:

$$R(E) = 10^{B(E)} \tag{3}$$

$$B(E) = p_{10} + \sum_{i=1}^{9} p_i \times [\log_{10}(E)]^{10-i} \tag{4}$$

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Table 1
Fitting coefficients p_1 to p_{10} corresponding to Eqs. (3) and (4) for the behavioral modeling of the LET versus ion energy.

Ion	p_1	p_2	p_3	p_4	p_5	p_6	p_7	p_8	p_9	p_{10}
$^{1}_{1}$H	−0.000072	0.000313	0.000801	−0.005735	0.004161	0.016050	−0.058306	0.172295	1.508268	1.212035
$^{2}_{4}$He	0.000230	−0.001294	−0.001047	0.015509	−0.005743	−0.086562	0.074551	0.364402	0.937028	0.546634
$^{3}_{6}$Li	−0.000228	0.000661	0.002999	−0.005415	−0.025006	0.004855	0.149170	0.157453	0.727124	0.420795
$^{4}_{8}$Be	0.000285	−0.001407	−0.000455	0.011422	−0.016504	−0.029281	0.140768	0.118997	0.655164	0.337527
$^{5}_{10}$B	0.000505	−0.002682	−0.000231	0.019618	−0.023021	−0.036910	0.139100	0.076552	0.668135	0.228816
$^{6}_{12}$C	0.000408	−0.002376	0.000552	0.017223	−0.025489	−0.027506	0.140963	0.033676	0.642289	0.194686
$^{7}_{14}$N	0.000354	−0.002357	0.001813	0.015679	−0.031779	−0.015370	0.145143	−0.011943	0.636229	0.161748
$^{8}_{16}$O	0.000037	−0.000902	0.003432	0.003016	−0.032759	0.024607	0.140068	−0.081166	0.628646	0.164015
$^{9}_{18}$F	−0.000045	−0.000707	0.004194	0.002069	−0.035774	0.024161	0.143401	−0.085871	0.615726	0.132176
$^{10}_{20}$Ne	−0.000022	−0.000764	0.003949	0.001845	−0.032257	0.029588	0.121298	−0.118845	0.644585	0.145051
$^{11}_{22}$Na	−0.000085	−0.000196	0.003569	−0.003571	−0.027971	0.053294	0.111525	−0.178127	0.645318	0.163270
$^{12}_{24}$Mg	−0.000132	−0.000110	0.004453	−0.005289	−0.032196	0.063200	0.114376	−0.207351	0.647418	0.164492
$^{13}_{26}$Al	−0.000162	0.000257	0.003401	−0.007000	−0.021882	0.061737	0.078688	−0.196060	0.693492	0.120705
$^{14}_{28}$Si	−0.000305	0.000815	0.004645	−0.013059	−0.023557	0.081572	0.066732	−0.208296	0.721947	0.047830
$^{15}_{28}$P	−0.000224	0.000467	0.003608	−0.007899	−0.019252	0.056598	0.056851	−0.167203	0.731879	0.019093

where coefficients p_i corresponds to a set of 10 real coefficients for each given ion.

Considering Eqs. (1)–(4), the proposed solution then requires to determine a unique set of 34 reals per given ion and per given target to analytically describe both LET(E) and $R(E)$ relations in the full energy range [1 keV, 1 GeV]. In order to calculate such coefficients, we developed a dedicated Matlab® macro[2] that minimizes the numerical error between SRIM data and analytical representations. Briefly, this script creates a data structure for the fit using the Matlab® "fitoptions" function [4] that specifies information like weights for the data, fitting types ("sin8" for Eq. (2), "poly9" for Eq. (4)), fitting methods ("NonlinearLeastSquares") and other options for the fitting algorithm [4]. SRIM data are loaded into the structure directly from the reading and pre-processing of SRIM output files and, as the result, the script generates a text file with the 34 real fitting coefficients plus the evaluation of the minimum, maximum and averaged errors on the specified energy domain for each ion. The program can directly process several SRIM files in a single execution sequence, then directly providing a matrix of coefficients for a collection of ions and/or targets. The resulting set of coefficients can be directly copy and paste to create numerical functions in any programming language on the basis of Eqs. (1)–(4).

3. Results and discussion

We illustrate in the following the results of this behavioral modeling of SRIM tables for fifteen ions ranging from $^{1}_{1}$H to $^{28}_{15}P$ in a silicon target. This particular case is important for microelectronics since it corresponds to secondary ions that be produced from nuclear reactions between atmospheric neutrons and silicon [5], possibly inducing single event effects in circuits. Numerical simulation of such effects requires very frequent computation of stopping power and range of produced ions, fully justifying the present approach.

Tables 1 and 2, respectively gives the p_i and a_i, b_i, and c_i coefficients for the LET and the range of all these ions in silicon, as obtained from the processing of the corresponding SRIM output files (SRIM version 2012) with the Matlab® program (R2012a release). These coefficient values have then been implemented in C++ functions to generate continuous numerical data. Fig. 1 illustrates the comparison of both tabulated and modeled data for a few ions, demonstrating the excellent fitting of the SRIM values by Eqs. (1)–(4). In order to quantify the accuracy of these numerical representations, Fig. 2 shows the averaged error estimated by the Matlab® fitting routines for both LET and range in silicon of the different ions defined in Tables 1 and 2. The averaged error is less than 1.2% for LET and less than 1% for range for the selected ions, which confirms the very good accuracy of the proposed approach. This later has been also successfully tested for silicon dioxide and cupper target (data not shown) with numerical errors in the same order of magnitude, around or below the percent.

Finally, to validate our approach with a practical case, we implemented and used the developed numerical functions into the TIARA code for the simulation of soft errors induced by atmospheric radiation in static memories (SRAMs). TIARA (Tool suIte for rAdiation Raliability Assessment) is a general-purpose Monte Carlo program written in C++ that simulates the interaction of several particles (neutrons, protons, alpha-particles and heavy ions) with various architectures of electronic circuits [6–8]. The code was initially designed to directly import SRIM data and to linearly extrapolate range and LET values of secondary ions from SRIM tabulated values. In a recent study [9], the code was used to evaluate the soft error rate (SER) induced by atmospheric neutrons in three generations of SRAM circuits, respectively manufactured in 130 nm, 65 nm and 40 nm technologies. Fig. 3 shows a comparison of the SER values evaluated using the initial release of the TIARA code and a new version implementing the numerical functions for both LET's and ranges proposed in the present work. For both simulations, we considered 500×10^6 of incident neutrons distributed in energy following the reference atmospheric spectrum at ground level given in [10]. The SER results are found strictly equivalent for both versions of the code; the small differences are only attributable to numerical fluctuations usually observed in the Monte Carlo simulation method from a simulation run to another.

4. Conclusion

In summary, we proposed in this work a behavioral modeling of SRIM tabulated data in the form of fast and continuous power polynomial fitting functions for the stopping power and projected range versus particle energy. A dedicated automatic procedure has been also developed under Matlab® to calculate the polynomial coefficients by minimizing the error between the data to model and the numerical representation. Typical accuracy below the percent has been obtained in the range 1 keV–1 GeV for a wide variety of ions and targets. Finally, we successfully tested and implemented the proposed solution for the case of secondary ions

[2] This macro is available for free download at the following URL: http://www.natural-radiation.net (top menu "Modeling/Simulation", section "SRIM Table Modeling").

Table 2
Fitting coefficients (a_1, b_1, c_1) to (a_{10}, b_{10}, c_{10}) corresponding to Eqs. (1), (2) for the behavioral modeling of the range versus ion energy.

Ion	a_1 b_1 c_1	a_2 b_2 c_2	a_3 b_3 c_3	a_4 b_4 c_4	a_5 b_5 c_5	a_6 b_6 c_6	a_7 b_7 c_7	a_8 b_8 c_8
$^{1}_{1}$H	1.956220	0.827775	0.097947	0.148241	0.086313	0.001234	0.001723	0.000541
	0.323238	0.850600	2.794768	3.495576	3.772755	6.184156	7.263390	8.850405
	−2.247633	1.823258	−2.611099	−0.118307	2.745605	−1.591242	0.886562	−3.689021
$^{2}_{4}$He	1.343970	1.161264	0.189282	0.001706	0.008809	0.005177	0.001628	0.000281
	0.515700	1.028412	1.803855	3.932618	5.006213	5.685879	7.087200	8.438661
	−2.445174	1.035452	−3.027577	−0.152822	2.256803	−1.623921	1.013650	−3.124702
$^{3}_{6}$Li	0.807533	0.652014	0.110944	0.036488	0.021734	1.776972	1.768770	0.001840
	1.205272	0.580013	2.121241	3.623005	4.845533	6.115976	6.120922	8.691919
	0.903794	−2.720591	3.344983	−0.192994	2.313348	−1.296632	1.842873	−2.605091
$^{4}_{8}$Be	2.218317	1.571908	0.390005	0.012631	0.017044	0.005777	0.002627	0.001935
	1.329730	1.430394	0.535122	3.848398	4.906220	6.234944	7.500284	8.837898
	0.725164	−2.488038	3.275295	0.756920	1.935856	−1.438986	1.015901	−2.877071
$^{5}_{10}$B	4.086886	3.649270	0.010275	0.017128	0.026199	0.010496	0.010002	0.006215
	0.776971	0.725456	2.725142	5.262824	3.893906	6.657418	7.739144	8.276188
	0.684197	3.729080	−0.912435	1.836107	1.346917	−2.459317	−0.167626	2.634144
$^{6}_{12}$C	0.872859	0.533693	0.007681	0.027130	0.012006	0.007783	0.007509	0.005588
	0.916953	0.744836	2.678857	3.842144	5.170452	6.624791	7.943302	8.608565
	0.486781	2.758709	−1.355789	1.085322	1.773573	−2.377272	−0.204121	2.452943
$^{7}_{14}$N	0.714216	0.132630	0.032608	0.007397	0.018223	0.015762	0.001915	0.009392
	0.790150	1.382951	3.754745	2.517784	5.242180	6.674428	13.774456	7.150627
	1.175368	−0.142722	0.917596	−1.908563	1.423563	−3.010529	1.123507	−0.277629
$^{8}_{16}$O	0.709179	0.188903	0.031090	0.011392	0.014088	0.003956	0.003201	0.001512
	0.731914	1.236427	3.540927	2.411203	4.667325	7.234530	7.884317	11.363786
	1.133574	0.040294	0.455165	−1.348325	0.903043	−3.165647	−0.348409	3.508969
$^{9}_{18}$F	0.765294	0.177953	0.038004	0.010038	0.031058	0.006750	0.028665	0.005273
	0.682119	1.310367	3.804492	2.530653	6.917037	4.448031	7.222415	11.388164
	0.998941	0.212229	0.329324	−2.918651	−3.391312	2.838901	−0.633313	2.976188
$^{10}_{20}$Ne	0.617390	0.358670	0.036321	0.023972	0.019304	0.039577	0.036053	0.004802
	0.574873	1.107210	3.802612	2.535185	4.860104	6.875954	7.069492	11.408358
	1.022313	0.369183	0.129087	−2.683918	1.399990	1.620334	−1.817266	2.236381
$^{11}_{22}$Na	0.878029	0.158675	0.023183	0.026452	0.025415	0.019122	0.093455	0.092681
	0.686509	1.271184	3.993324	5.811342	6.022104	2.598439	10.800094	10.767664
	0.850637	−0.191131	0.199708	0.712431	3.615855	−0.293170	2.689499	−0.415540
$^{12}_{24}$Mg	0.952986	0.134501	0.029698	0.063492	0.060289	0.963900	0.055281	0.909693
	0.666869	1.511807	3.844329	5.805575	5.978005	11.377166	11.067628	11.395236
	0.726381	−0.118447	0.071261	0.401430	3.350518	1.509906	−1.309931	−1.650419
$^{13}_{26}$Al	0.938132	0.173064	0.021520	0.004522	0.008647	0.004948	0.004149	0.002828
	0.628930	1.280560	3.903995	5.057902	3.113949	7.660582	6.996557	8.708039
	0.795827	−0.211745	0.065100	0.951061	−1.419880	2.476814	0.625648	−1.803427
$^{14}_{28}$Si	1.056648	0.026705	0.026059	0.152847	0.014583	0.008291	0.004048	0.002263
	0.633748	2.515204	3.774124	1.273392	5.068415	6.294246	7.667861	8.834262
	0.888116	−0.688891	0.104702	−0.918549	0.121050	1.149604	2.023986	−2.358316
$^{15}_{28}$P	1.093973	0.137012	0.016655	0.012632	0.006995	0.007014	0.002935	0.001869
	0.633742	1.265217	3.801339	5.068163	6.336489	2.515705	7.604467	8.869279
	0.850780	−1.005518	0.200337	−0.379640	0.962197	−1.031704	2.021591	−2.623060

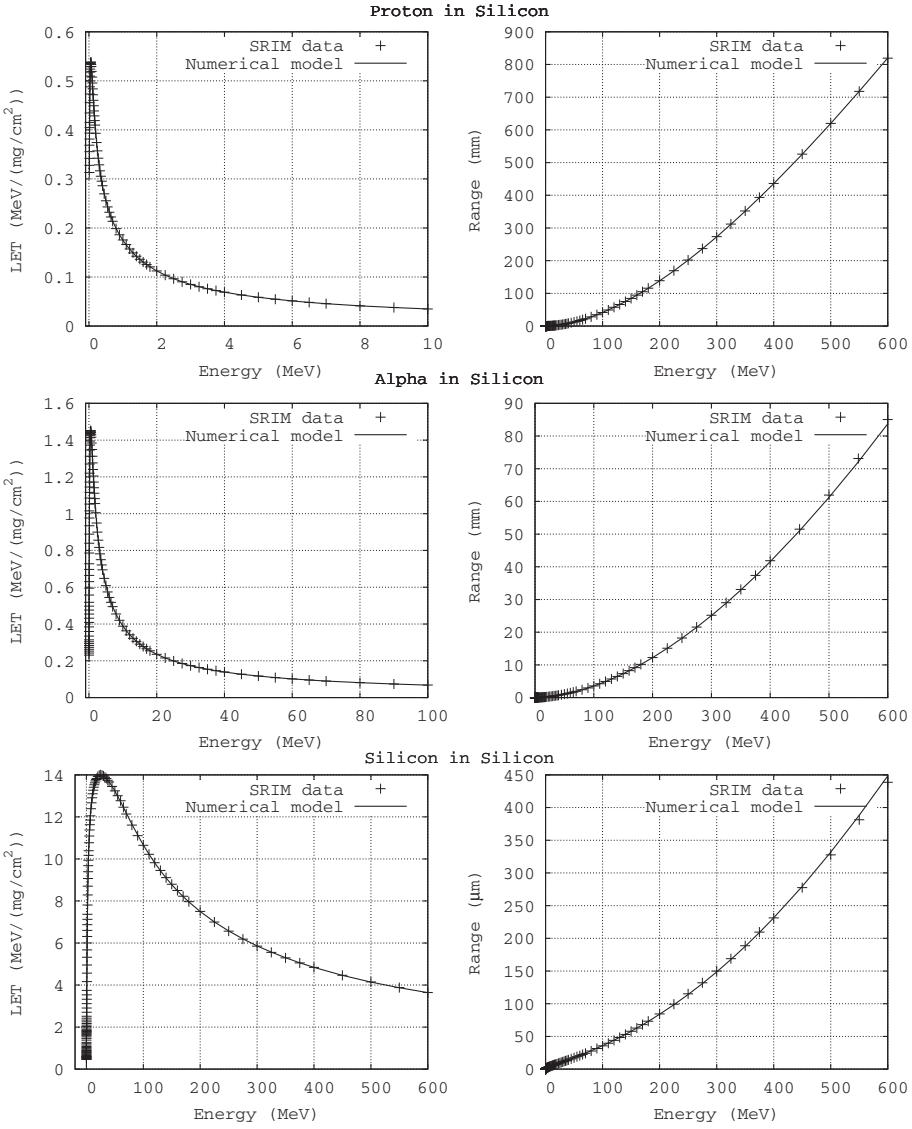

Fig. 1. Comparison between SRIM data and numerical values (LET and range) calculated using the approximation functions for protons, alphas and silicon ions in silicon target as a function of ion energy.

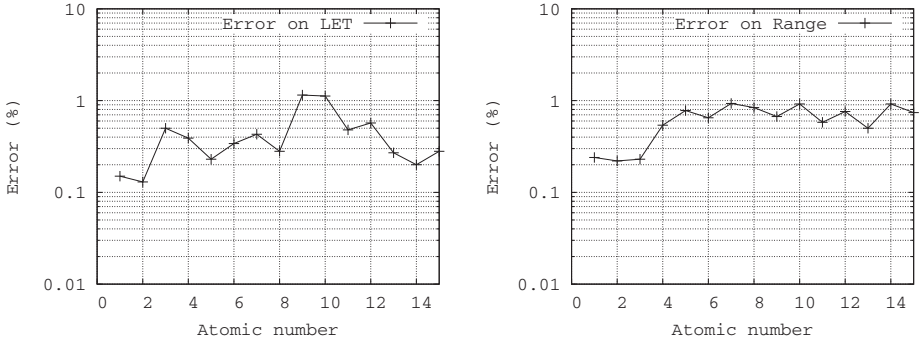

Fig. 2. Numerical averaged error between SRIM data and values calculated using the approximation functions for both LET and range in silicon as a function of the atomic number of the ions defined in Tables 1 and 2.

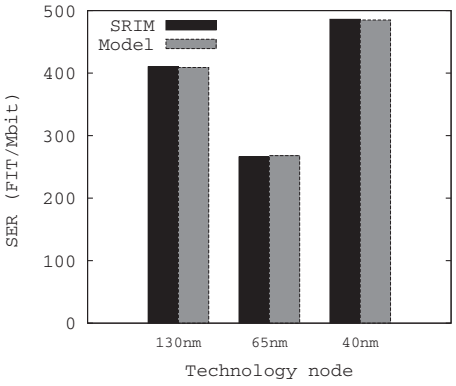

Fig. 3. Soft error rate (SER) values computed by the TIARA simulation code for three generation of SRAM memories (see details in [9]) when directly considering SRIM tabulated data (SRIM) or using the approximation functions developed within this work (model).

(ranging from protons to silicon ions) produced from nuclear reactions between neutrons and the silicon bulk material of micro-electronics circuits.

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