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COMMENTS ON DPA CALCULATION METHODS FOR ION BEAM DRIVEN SIMULATION IRRADIATIONS

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The methodology of application of computer simulation technique to the NSC KIPT advanced simulation studies of radiation materials science at charged particles accelerators is considered with due account of the conformance of simulation methods and algorithms to the working standards of nuclear engineering. The ambiguities of dpa calculations by means of the SRIM code are demonstrated and analyzed using complementary simulations by means of the RaT Monte-Carlo code. The refined guideline of the SRIM dpa calculations is presented.

1. INTRODUCTION

Ion beam simulation irradiation of structural materials is used in NSC KIPT [1–3] and worldwide [4] as a valuable technique of express assessment of their radiation stability under nuclear reactor (n,γ) irradiation. The established standard practice of simulation studies [5] prescribes the calculation of the number of atomic displacements per atom (*dpa* defined [5] as "*a unit of radiation exposure giving the mean number of times an atom is displaced from its lattice site*") as an adopted metric of correlation of the radiation damage relevant effects in metals and alloys subjected to different irradiation environments. This allows comparison of the results of accelerator and reactor based irradiations as well as of those of different experimental groups [4, 5].

The quantification of spatially dependent dpa is a complicated radiation transport problem mostly solved by means of the Monte Carlo (MC) modeling software. The SRIM package [6] is a publicly available [7] practically standard [5] user-friendly tool of such kind of calculations applicable to ~$10^{(0...4)}$ keV ion beams irradiation of planar layered targets. The TRIM MC code of the SRIM package simulates depth profiles of irradiation induced vacancy-interstitial Frenkel pairs (FPs) using the binary collisions approximation (BCA) method. Under the assumption that each FP arises in a single atomic displacement, a common practice is to scale dpa at a given ion fluence Φ, cm^{-2}, with the vacancy profile the TRIM code outputs in the VACANCY.TXT file.

The present paper addresses the known issue of this code application to dpa calculations. TRIM offers two options for the FP distributions simulation. The express *"quick damage"* (QD) method simulates only the trajectories of primary ions and the production of primary knock-on atoms (PKAs). The total FP production rate is then calculated analytically within the scope of the modified Kinchin-Pease (K–P) [8, 9] model of the secondary displacement function (SDF) $\nu(T)$, the number of the secondary knock-on atoms (SKAs) produced by a PKA of energy T at a user-supplied value of a stable FP production threshold energy E_d. The alternative *"full cascades"* (FC) damage MC simulation method simulates the overall collision cascade explicitly down to certain cut-off energy $E_{fin} \sim 1$ eV of BCA applicability. The numbers of FPs and atomic replacements are scored collision-by-collision according to certain decision rules based on the values of E_d and the lattice binding energy E_b.

The issue consists in the about twofold discrepancy of the vacancies (and thus dpa) profiles simulated by means of the FC and QD methods (Fig. 1). The ratio is too high to rate it as a reasonable scattering of the estimate of the same physical quantity. It is very probable that the FC/QD methods deviate systematically.

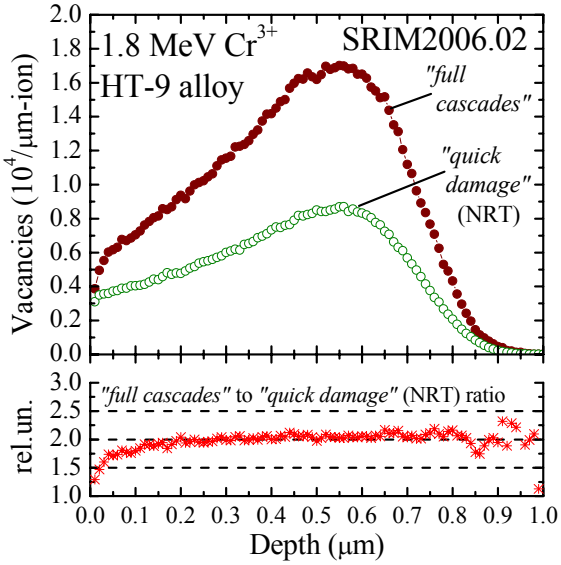

Fig. 1. Depth profiles of the total number of vacancies produced under irradiation of ferritic-martensitic steel HT-9 by 1.8 MeV Chromium ions at the NSC KIPT ESUVI accelerator [2] as calculated using two alternative damage simulation methods of the TRIM BCA code

Neither SRIM manuals [7] nor the ASTM simulation standard [5] comment the origin of this difference. The TRIM simulation method (FC/QD) is seldom specified in publications of experimentalists. This is fraught with misinterpretation of the measured irradiation effect (*e.g.* swelling) in terms of the calculated dpa, *esp*. significant for the topical case of ultra-high (300…600 dpa) damage dose irradiation [2] of prospective reactor materials.

The goals of the present paper are: (i) to uncover physical and algorithmic reasons of the observed discrepancy and (ii) to refine a guideline of the dpa rate calculations by means of the TRIM BCA code.

In sec. 2, we outline the meaning of dpa in radiation material science (RMS) R&D and the methods/models implemented in various codes (*incl.* TRIM) for dpa calculations. Since TRIM is not an open-source software, certain fine details of its algorithms (the calculated dpa seem to be sensitive to) are only poorly documented in [6,7,10] and subjected to changes from one version of the code to another. However, they are extractable from

the deep analysis of the code operation. This way is adopted in sec. 3. Here we present the novel SRIM compatible modification [11] of the in-house developed CERN GEANT4 Toolkit [12] based multi-purpose MC code RaT 3.1 [13] and show its capability of reproduction of TRIM FC/QD simulations of both damage profiles and SDF. We juxtapose them with the controllable algorithms of the RaT code and give a quantitative measure of the procedural sensitivity of dpa calculations. In sec. 4, this grounds the conclusions on the preferred options of SRIM dpa calculations in conformity to the working standard [5] of ion beams driven RMS simulation studies. We end the paper with the prospects of further developments in view of recent IAEA supported activities [14] directed toward the long-expected refinement of radiation damage simulation standards.

2. A SURVEY OF DPA CALCULATION METHODS AND SOFTWARE

When applying computer codes to the RMS relevant studies, one should clearly distinguish between the simulations of radiation damage and dpa. These physically closely related problems differ methodologically.

The ultimate goal of the radiation damage simulation is an *ab initio* prediction/explanation of the observed changes of macroscopic properties of irradiated materials (swelling, creep, embrittlement, stress corrosion cracking, *etc.*). The regularities of these phenomena are very complicated [1, 4] subject to the kind (neutrons, ions, electrons), intensity, energy spectrum, temperature and stress conditions of irradiation as well as to the evolving chemistry (nuclear transmutation) and microstructure of materials (vacancies and self-interstitial atoms (SIA) recombination and annealing, diffusion and clustering, nucleation and evolution of voids, precipitates and dislocation loops). The driving forces of these changes spread over an extremely broad time scale starting from the primary development and athermal quenching of displacement cascades ($\sim 10^{-(13\ldots11)}$ s) [15] through the kinetic stage of short-term ($\sim 10^{-(11\ldots6)}$ s) defects recovery up to the rate theory [16] described diffusion stage ($>10^{-6}$ s) of structural and phase transformations. By reason of a limited computer power, it is out of the current agenda to integrate the models of all theses stages into a self-consistent software. Instead, the coherent concept of multiscale modeling [1, 4, 14–16] of radiation damage is developing for harmonization of inputs and outputs of successive tiers of simulation codes. Among them, only the earliest ballistic stage (~ps) deals with dpa relevant atomic displacements well described by the stable molecular dynamics (MD) [15]. The most computationally efficient BCA method of the MARLOWE [17] or TRIM codes is in fact the extremely degenerated MD. Later the Recoil Interaction Approximation MD (RIA-MD) was proposed [18] to upgrade BCA toward an adequate treatment of collective lattice-driven effects (focusing, channeling) without visible loss of efficiency. RIA-MD software (like our MICKSER code [19]) is capable of precise atomistic calculations of ion induced dpa rates.

However, the principal application of the dpa concept is far from such an atomistic modeling. It covers the routine tasks of nuclear reactor dosimetry of radiation damage [1, 4, 14] by means of the industry-grade MC codes like MCNP(X), MCU, MVP, KENO, *etc*. Such codes succeed in detailed 3D calculations of neutron and gamma fluxes inside and beyond a reactor core but do not attempt to simulate displacement cascades atomistically. The atomic displacements are considered "parasitically" as a particular case of primary irradiation induced secondary effects of finite microscopic cross-sections. The dpa rate is calculated as follows:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{dpa}(\mathbf{r}) = n \cdot \sum_i \int_{E_i} \phi_i(E_i;\mathbf{r}) \cdot \sigma_{\mathrm{D}}^{(i)}(E_i)\,\mathrm{d}E_i \ , \qquad (1)$$

where n (atoms·cm^{-3}) is the number density of a material, i enumerates the kind of primary radiation, ϕ is the energy E spectrum of the correspondent MC simulated flux (cm^{-2}·s^{-1}) in a point $\mathbf{r}$, σ_{D} is the effective cross-section of displaced atoms production by each specific kind of radiation. The latter function is in turn a convolution of the PKA energy T spectrum σ_{PKA} and the SDF ν

$$\sigma_{\mathrm{D}}(E) = \int_{E_{\mathrm{d}}}^{T_{\max}(E)} \sigma_{\mathrm{PKA}}(T,E) \cdot \nu(T)\,\mathrm{d}T \qquad (2)$$

over the whole range of T above the production threshold E_{d}. The MC code applies the precomputed damage-energy cross-sections $2E_{\mathrm{d}} \cdot \sigma_{\mathrm{D}}(E)$ (eV·barn) which are practically independent on E_{d} (at least for neutrons) and are also referred as the displacement kerma factors. They are calculated off-line from the evaluated nuclear data by the data processing software (*e.g.*, the HEATR module of the NJOY package [20]). Besides, the displacement kerma databases are incorporated into the widespread end-user utilities (like ENDF/B-V based code SPECTER [21] or the JENDL based code NPRIM [22]) for express calculations of dpa in reference neutron environments of different nuclear reactors.

Within this approach, the dynamics of displacement damage is concentrated in the model representation of the SDF $\nu(T)$ thus omitting all the above-mentioned diversity of primary irradiation effects and reducing them to the production of elementary point defects (FPs). This is inherited from the very early stage of radiation damage theory (prior to the disclosure of swelling or radiation induced segregation) considered FPs as the only consequence of irradiation. The simplicity of this assumption gave rise to a set of exactly solvable models. For instance, the elementary balance equation

$$\int_0^T P(\tau) \cdot \left[\nu(\tau) + \nu(T-\tau) - \nu(T)\right] \mathrm{d}\tau = 0 \qquad (3)$$

with the hard-sphere energy transfer p.d.f. $P(\tau)\mathrm{d}\tau = \mathrm{d}\tau/T$ and the boundary conditions $\nu(E_{\mathrm{d}}) = 0$, $\nu(2E_{\mathrm{d}}) = 1$ yields

$$\nu_{\mathrm{KP}}(T) = \begin{cases} 0, & T < E_{\mathrm{d}}, \quad (4.1) \\ 1, & E_{\mathrm{d}} \le T \le 2E_{\mathrm{d}}, \quad (4.2) \\ T/2E_{\mathrm{d}}, & 2E_{\mathrm{d}} < T \le E_{\mathrm{c}}, \quad (4.3) \\ E_{\mathrm{c}}/2E_{\mathrm{d}}, & T > E_{\mathrm{c}}, \quad (4.4) \end{cases}$$

where E_{c} is the upper cut-off energy of discrimination of elastic ($T < E_{\mathrm{c}}$) and inelastic (i.e. electronic, $T > E_{\mathrm{c}}$) energy losses of cascade atoms. Eq. (4) was first obtained by Kinchin and Pease in 1955 [8]. Numerous refinements of the K–P model were obtained in 1960-70s with the more accurate account for the detailed energy balance, the anisotoropy of screened Coulomb scattering,

the realistic partitioning of nuclear and electronic stopping and the impact of directional effects of channeling and focusing (see chap. 2 of ref. [2] for further details). In general, the predictions of all these models were found to scatter within ~100%. For practical purposes, this stimulated the elaboration, in 1975, of the synoptic model of SDF known as the NRT standard [9].

Norgett, Robinson and Torrens [9] proposed the following general form of SDF:

$$\nu_{\mathrm{NRT}}(T) = \kappa \frac{E_{\mathrm{D}}(T)}{2E_{\mathrm{d}}}\ , \qquad (5)$$

where $\kappa = 0.8$ is the PKA mass and target temperature independent efficiency factor following from the atomic scattering anisotropy in the screened interaction potential. Its value (0.8) was obtained as an appropriate fit of the results of a series of MARLOWE BCA code calculations undertaken for Cu, Fe, Au and W targets [17]. For $T > 2E_{\mathrm{d}}/\kappa$, it was found to be the PKA energy independent while $\kappa = \kappa(T)$ due to lattice-driven effects at lower T. The $E_{\mathrm{D}}(T)$ is the "damage energy" (or the "non-inelastic energy loss", NIEL) available to produce displacements. To obtain it, the total electronic energy loss in a cascade is subtracted from the PKA energy. The standard adopts Robinson's parameterization to the LSS [23] energy loss partitioning function. This yields

$$E_{\mathrm{D}}(T) = \begin{cases} 0, & T < E_{\mathrm{d}}, \qquad (6.1) \\ \dfrac{2E_{\mathrm{d}}}{\kappa}, & E_{\mathrm{d}} \le T \le \dfrac{2E_{\mathrm{d}}}{\kappa} = 2.5E_{\mathrm{d}}, \qquad (6.2) \\ \dfrac{T}{1 + k_{\mathrm{L}} g(\varepsilon)}, & T > \dfrac{2E_{\mathrm{d}}}{\kappa}, \qquad (6.3) \end{cases}$$

where $\varepsilon = a_{\mathrm{TF}} T / 2(Ze)^2$ is the Lindhard's reduced energy of PKA with atomic and mass numbers Z and A, respectively, $a_{\mathrm{TF}} = 0.6262 Z^{-1/3} a_{\mathrm{B}}$ is the screening length, a_{B} is the Bohr atomic radius, $k_{\mathrm{L}} = 0.1337 Z^{1/6} \sqrt{Z/A}$ and $g(\varepsilon) = \varepsilon + 0.40244\varepsilon^{3/4} + 3.40086\varepsilon^{1/6}$. The formulae emphasize that this treatment is a particular case of LSS theory rigorously applicable only to a single-component material. When applying to multi-component materials, effective Z and A and the same value of the threshold energy E_{d} shall be used for all atomic species (typically, E_{d} = 40 eV for structural steels and alloys).

These limitations of the NRT standard are evident. Much more serious restrictions cover the disregard of recombination, subcascades and other effects which appear in MD modeling and essentially determine the displacement efficiency [15, 24]. Now the ~40 years old NRT standard looks outdated and shall be revised and upgraded in the near future [14]. However, its merit consisted in a closed, simple, and general form equally suitable for both analytical calculations and implementations into computer codes. As a result, all industry-standard reactor MC codes make use of the NRT standard displacement model to calculate dpa. They differ only in the SDF treatment details in the vicinity of E_{d}.

Let's summarize the difference of the considered approaches with the following intermediate conclusions. An atomistic MD, RIA-MD and BCA simulations attempt to model atomic displacements and radiation defects in materials as close as possible to the experimentally observed picture. From the other hand, dpa calculated by the computational dosimetry relevant software is never observable experimentally. Currently it has the exclusive meaning of the NRT standard supplied dosimetric quantity, a conventional unit of measurement of irradiation impact. Just in this sense NRT dpa is mentioned in the ASTM standard practice [5]. The physical adequacy of NRT dpa is thus of less value then the coherence of their use in different simulation studies.

3. INTERROGATION OF THE TRIM CODE DPA CALCULATIONS ALGORITHMS

To rationalize the observed behavior of the FC/QD algorithms (see Fig. 1), we perform calculations in parallel by means of the TRIM and RaT 3.1 codes. Similar to NJOY/MCNP, the RaT can calculate and use nuclear heating and displacement kerma factors for reactor dosimetry relevant MC simulations [25]. Their NRT standard (5–6) specific version is compared with the QD options of TRIM. Moreover, RaT is currently the only general-purpose MC 3D radiation transport code capable of explicit atomistic BCA modeling of collision cascades [11] using the "universal" Ziegler-Biersack-Littmark (ZBL) interaction potential and the electronic stopping power database of the SRIM package [6] (for details, see [11]). At its validation [11], the TRIM FC SDFs for He, Ni, and Xe irradiation of Nickel were reproduced within ~5% in a broad range of energies. Thus the RaT's "explicit cascade" mode is expected to qualify the FC mode of TRIM. In fact, Fig. 2 clearly shows an excellent agreement of the results of TRIM and RaT calculation for both FC and QD modes of TRIM.

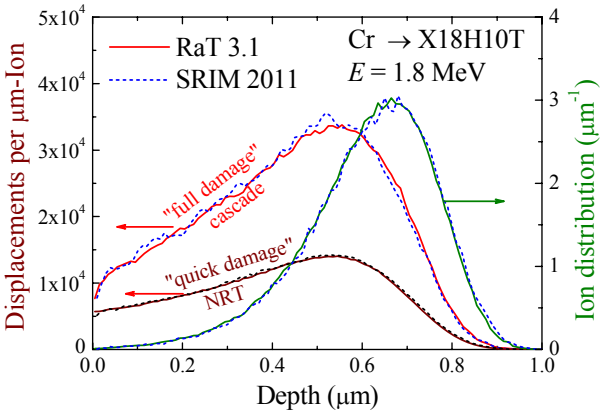

Fig. 2. Doping and damage profiles calculated for the case of the simulation irradiation [3] using the FC and QD options of TRIM (dotted curves) and the appropriate algorithms of the RaT MC code (solid curves) [11]

The difference between QD/FC simulated damage profiles (see Figs. 1, 2) is not only inherent to irradiations by heavy ions. The RaT code simulates radiation damage produced in 3D targets by a great variety of primary radiations (n, p, α, $e^{\pm}$, γ) with complex energy spectra. Fig. 3 [11] shows that the ~50 % difference of the explicitly calculated and NRT predicted dpa profiles also takes place at materials irradiation by relativistic electrons of the NSC KIPT LPE-10 linac.

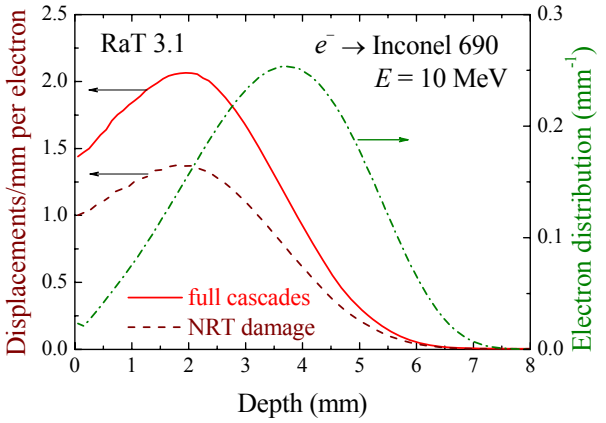

Fig. 3. Deposition and damage profiles of the LPE-10 linac 10 MeV electrons in a slab of Ni–Cr alloy 690. A comparison of the explicit and NRT models predictions

Fig. 4 clearly demonstrates that the FC/QD discrepancy is common to the overall topical range of PKA energies (from E_d = 40 eV up to 2 MeV) where the SDFs ν in Iron calculated using both codes are well agreed. It is evident that the QD option is in the closest agreement with the predictions of the NRT standard SDF (5, 6). For FC mode, the deviation arises in the TRIM data extracted from the VACANCY.TXT file (N_v, the number of vacancies) and in the summarized number of atomic displacements: $N_d = N_v + N_r$ where N_r is the total number of atomic replacements per PKA (a file NOVAC.TXT).

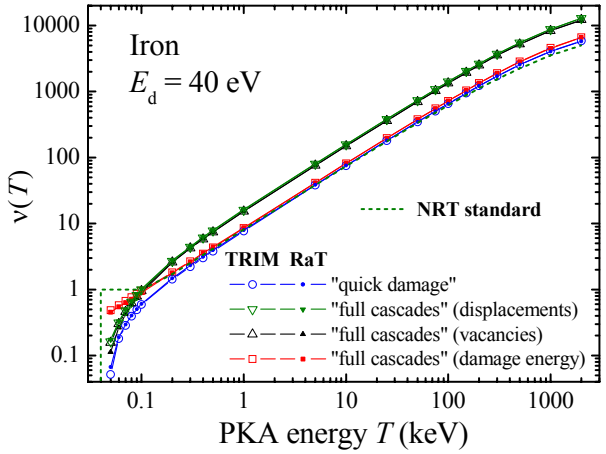

Fig. 4. PKA energy dependencies of the SDF in Iron calculated using various methods of the TRIM BCA (open markers) and RaT 3.1 MC (bold markers) codes as compared to the NRT standard SDF (dashed curve)

However, there exists an undocumented way to obtain the NRT compatible data from the results of TRIM FC modeling. The non-ionizing energy losses of PKA and SKA are after all dissipated to phonons. TRIM accumulates them in the PHONON.TXT file as a function of depth. Obviously, these data represent the profile of NIEL or damage energy E_D. Thus one can calculate the SDF (5) directly from the PHONON.TXT data without reference to the LSS partitioning function (6). The results are tagged in fig. 4 as a "damage energy" method. RaT uses NIEL to obtain the compatible data.

The data of Fig. 4 are normalized to the NRT SDF (5–6) in Fig. 5. Here one can see that RaT reproduces all SRIM data to a few percents relative precision. NRT-based models (QD and damage-energy/NIEL) deviate from the standard values not more then by 10…20 % for all energies of interest (T > 100 eV). However, the FC-based methods manifest in this range of T the energy dependent 200…250 % high excess over the NRT standard. Now we focus on the origin of this deviation.

Note that it well agrees with the ratio (=2) of the mean number (T/E_d) of displacing collisions and the K–P model (4.3) predicted number of FP, $T/2E_d$. One should be aware that both K–P and NRT models counts vacancies (or FPs), but not displacements. The difference between them falls on replacement collisions (in TRIM, displacements = vacancies + replacements [7]).

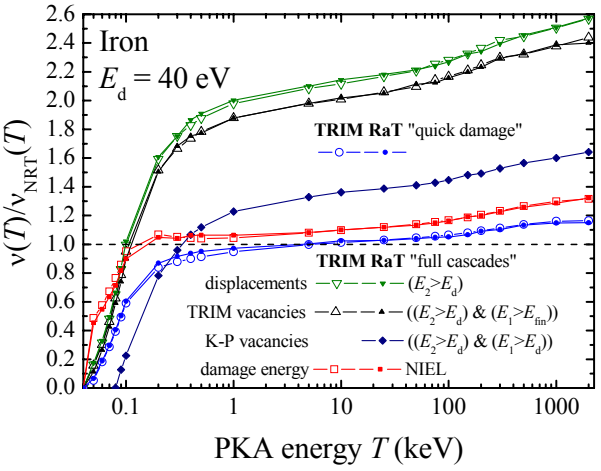

Fig. 5. The ratios of the simulated and NRT SDFs of Iron according to the data of Fig. 4

The FC algorithm scores displacements, vacancies and replacements by the analysis of energy transfers at each binary collision in a cascade. It apply energy-based criteria to identify the type of produced damage. Suppose $E_{1,2}$ are the energies of scattered and struck atoms after a collision. TRIM [7] (as well as MARLOWE [17] and other BCA codes) identifies displacement if $E_2 > E_d$ irrespectively of E_1. The K–P model (4) produces a vacancy from displacement only when $E_1 > E_d$. This is the meaning of the boundary condition $\nu(2E_d) = 1$ of Eq. 3. Otherwise ($E_1 < E_d$) the vacancy is immediately annealed by the incident atom, and the replacement occurs. This scenario corresponds to the "K–P vacancies" curve of Fig. 5 obtained by the RaT code modeling. Evidently, it strongly deviates of the "TRIM vacancies" data.

TRIM manuals (SRIM-08, p. 8-10, SRIM-09, p. 9-34 [7]) declare the conformity of the replacements identification rule to the above described K–P scenario and supplement it with the condition of identity of scattered and struck atoms (K–P was written for a single specie case). However, page 3 of the SRIM Tutorial 4, "Target Damage" states the another replacement rule, $E_1 < E_{fin}$ where $E_{fin} << E_d$ is the cut-off energy of moving atom "below which it is considered to be stopped". The specific value of $E_{fin} \sim 1$ eV is undocumented and cannot be accessed or altered by users. Moreover, it seems to be material specific. RaT fits TRIM at E_{fin} = 4 eV for Iron.

Therefore, the excess of vacancy production rate is mainly caused by the underestimation of replacements with respect to those assumed in K–P model and NRT.

In comparison with the requirements of the NRT standard, the working version of the TRIM FC algo-

rithm tries to simulate the collision cascade in much more details. Sub-threshold atoms can leave a vacancy when they escape from the target surface. Therefore, SRIM FC simulations are self-consistent. However, the concerned user must be aware that the FC produced "TRIM vacancies" are not the same that the "NRT dpa".

It is very probable that the correlation of this metric with the experimentally observed irradiation effects should be not worse then the NRT dpa. Fig. 6 shows that the ratios of the FC calculated SDFs (explicit to effective damage energy derived) is only a weak function of PKA energy. Thus, "TRIM vacancies" (or "TRIM FC dpa") is simply an another unit of measurement.

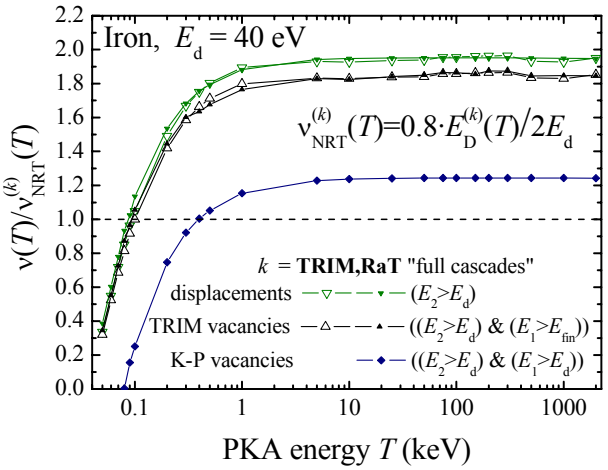

Fig. 6. The SDF ratios calculated using the algorithms of explicit cascade modeling and the NRT-compatible methods of damage energy calculation

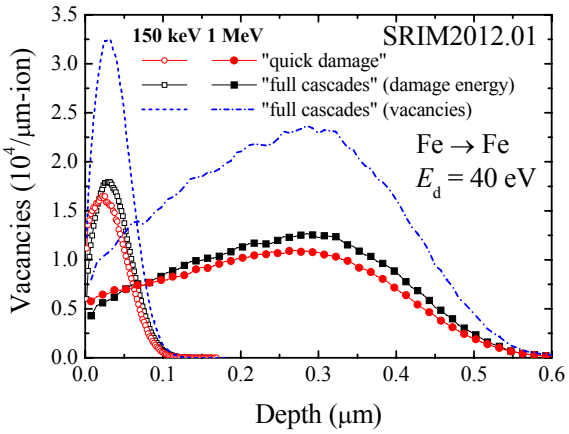

Fig. 7. The TRIM calculated damage profiles for 150 keV and 1 MeV Fe self-ions irradiation of Iron

The FC "damage energy" metric (that follows from the analysis of the PHONON.TXT file) can provide experimentalists with (almost) NRT-compatible data on dpa profiles (Fig. 7). Since ion-target interactions are simulated more accurately in the FC mode, this can improve the prediction of the expected dpa profiles at planning of ion beam simulation irradiation, especially with multi-component targets.

4. CONCLUSIONS

The SRIM package is a well approved and powerful tool suitable for atomistic simulation of ion beam interaction with solid, ion implantation, sputtering, and the production of radiation defects. However, when applied to the reactor materials science relevant computational dosimetry of ion beam driven simulation irradiations, it must be used with caution. The parameters and the settings of the BCA simulation have to be chosen accordingly to the specific goal of computer modeling and irradiation experiment, and should not be omitted in publications of simulation results.

Different regimes of the code operation output physically reasonable but semantically different dosimetric quantities. To compare with the reactor damage dosimetry data, the *"quick damage"* simulation option is the preferred one since its results are found to be the most closely conformant with the "NRT standard dpa" prescribed by the standard practice of simulation studies.

The application of other options deviates the results from the working standards. One is free to use them for "what-if" and sensitivity analyses. But an uncritical use of the *"full cascade"* option outputs can result in overestimation of the expected NRT dpa. This can be especially critical in the case of ultrahigh-dose irradiations when considering the dpa dependent threshold effects (*e.g.* swelling).

These conclusions are based on current regulations and are subject to change at the expected refinements of the NRT standard. The new generation GEANT4 based multi-purpose Monte Carlo radiation transport code RaT successfully reproduces the results of atomistic SRIM simulations. Due to its flexibility and capability of consistent simulation of coupled neutron-gamma, electron and ion beam relevant irradiations, it is a prospective platform for incorporation of new standards in the computational support of radiation materials science studies.

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ЗАМЕЧАНИЯ О МЕТОДАХ РАСЧЁТА С.Н.А. В ИМИТАЦИОННЫХ ОБЛУЧЕНИЯХ НА ПУЧКАХ ИОНОВ

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Методология применения методов компьютерного моделирования к развиваемым в ННЦ ХФТИ имитационным экспериментам радиационного материаловедения на ускорителях заряженных частиц рассмотрена с особым вниманием к соответствию методов и алгоритмов моделирования действующим стандартам атомной науки и техники. Продемонстрированы неоднозначности в расчетах с.н.а. средствами кода SRIM. Проведен их анализ путем дополнительного моделирования Монте-Карло-кодом RaT. Представлена усовершенствованная методика расчетов с.н.а. пакетом SRIM.

ЗАУВАЖЕННЯ ДО МЕТОДІВ РОЗРАХУНКУ З.Н.А. ЩОДО ІМІТАЦІЙНИХ ОПРОМІНЮВАНЬ НА ПУЧКАХ ІОНІВ

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Методологія застосування методів комп'ютерного моделювання до імітаційних експериментів радіаційного матеріалознавства на прискорювачах заряджених частинок, що розвиваються у ННЦ ХФТІ, розглянута з особливою увагою до відповідності методів й алгоритмів моделювання до діючих стандартів атомної науки і техніки. Продемонстровані неоднозначності у розрахунках з.н.а. засобами коду SRIM. Їх аналіз проведений шляхом додаткового моделювання Монте-Карло-кодом RaT. Представлена вдосконалена методика розрахунків з.н.а. пакетом SRIM.