Using SRIM to evaluate athermal recombination corrected displacement damage (ARC-dpa)

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In radiation damage studies, the need for quantitative comparison of experimental data acquired under different irradiation conditions led to the adoption of an international radiation exposure standard in terms of displacements per atom (dpa). The dpa parameter refers to the number of times a target atom is displaced from its lattice position, on the average, due to scattering by the bombarding particles. Kinchin & Pease [1] first proposed a model for calculating dpa, that was later modified by Norgett, Robinson and Torrens (NRT) [2] and it is now accepted as standard. The model takes into account the average target atom recoil energy and the displacement threshold of the given material. NRT-dpa is typically evaluated by means of specialized computer codes. In the case of ion irradiation, the SRIM code [3] is mostly employed for this purpose as previously documented [4].

However, a large number of experimental and theoretical studies have shown that the NRT model overestimates the induced damage, especially in the case of high energy events which result in atomic displacement cascades. In such events there is an increased probability of intra-cascade defect recombination due to the high kinetic energy of the displaced atoms. This effect, called "athermal recombination," leads to reduced numbers of stable displacements remaining after cascade cool-down. Recently, a correction of the standard NRT-dpa exposure calculation has been proposed, which takes intra-cascade recombination into account: the Athermal Recombination Corrected – dpa (ARC-dpa) [5]. This new damage model is not yet implemented in ion transport codes such as SRIM and, thus, its evaluation requires some post-processing by the user. In the current contribution we introduce a protocol for obtaining ARC-dpa values from SRIM output and present several examples over a wide variety of materials and ions.

[1] Kinchin, G. H., and Pease, R. S., *Reports on progress in physics*, V. 18, No. 1 (1955)
[2] Norgett, M. J., Robinson, M. T., and Torrens, I. M., *Nuclear Engineering and Design*, V. 33, No. 1 (1975)
[3] Ziegler, J. F., Ziegler, M. D., and Biersack, J. P., SRIM Co. (2008)
[4] Stoller, R. E., et al., *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, V. 310 (2013)
[5] Nordlund, et al., *Journal of Nuclear Materials*, V. 512 (2018)