

Calculations of Primary Damage with Binary Collision Approximation : dpa calculations and Iradina code

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Binary Collision Approximation is the basic tool to model damage and implantation profiles in ion irradiations. I will first present the Iradina code[1], which is a fast, user-friendly, open-source alternative to SRIM. Then, I'll discuss BCA damage calculations which are of two types : "Full cascade" or "Quick calculations". I'll recall what these two types of calculations are, their respective advantage and limitations. Recent improvements of both types of calculations will be presented :

-The arc-dpa damage function for the quick-calculations, an attempt to go beyond the NRT-dpa model [2];

-A correction to the full cascade simulations to reconcile them with the NRT calculations [3].

[1] https://sourceforge.net/projects/iradina/files/Iradina_CEA_GRAPHICAL_USER_INTERFACE/

[2] Nordlund, K., et al., Improving atomic displacement and replacement calculations with physically realistic damage models. Nature Communications, 2018. 9: p. 1084.

[3] Lin, Y.R., et al., Predicting displacement damage for ion irradiation: Origin of the overestimation of vacancy production in SRIM full-cascade calculations. Current Opinion in Solid State and Materials Science, 2023. 27.