Atomistic modelling of collision cascades for the integration of radiation damage in ReBCO superconductors for fusion

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With their reduced cost and building time, compact tokamaks promise to speed significantly up the road for affordable fusion energy. High Temperature Superconductors (HTS) have quickly become an enabling technology in the sector, thanks to the high magnetic fields that they can generate, cutting the size of the devices for a given plasma power [1][2]. However, the compactness introduces new challenges, enhancing the neutron irradiation on the magnets, introducing defects and structural modification able to degrade the superconducting properties and therefore reducing the lifetime of the system [3][4]. Considering the difficulties in reproducing this environment experimentally, computational methods can provide important insight into the microscopical mechanism underlying the degradation process, providing useful tools to design mitigating solutions [5].
In the present work we will show our effort in modelling damage processes in $YBa_2Cu_3O_7$ (YBCO) by means of molecular dynamics (MD) and binary collision approximation (BCA) simulations. For each of the possible primary knock-on atoms (PKA), several collision cascades were investigated for energies below 10 keV in MD, analysing the results in term of defects number and morphology. Accurate threshold displacement energies were than computed, considering the presence of different crystallographic sites, to access higher energies by means of BCA. Combined with integration over recoil spectra, the current approach will provide the basis for the calculation of radiation damage from atomistic simulations for any specific radiation environment.

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