The influence of electron-phonon coupling on the formation and distribution of defects during cascades

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Defect creation during irradiation leads to the long-term degradation of material properties. The exact mechanism of defect creation depends on the kinetic energy of the projectile and stopping power of the target material, with lower energy particles typically interacting with atomic nuclei, while at higher energies it is the electrons that become excited. Of particular interest for nuclear fusion is the region between these two regimes where both mechanisms are active simultaneously. In this domain energy transfer between ions and electrons through electronic stopping and electron-phonon coupling is predicted to have a substantial impact on the defect production. Two-temperature molecular dynamics (2T-MD) couples a traditional molecular dynamics supercell to a secondary subsystem representing the electrons that can mimic the exchange of energy between ions and electrons [1]. In this work, we explore the production of defects and their distribution for a series of different formulations of the 2T-MD model and demonstrate that schemes that neglect electron-phonon coupling during the very early stages of the cascade (< 0.2 ps), display markedly higher estimates of primary damage quantities with defects more likely to be found in larger clusters.

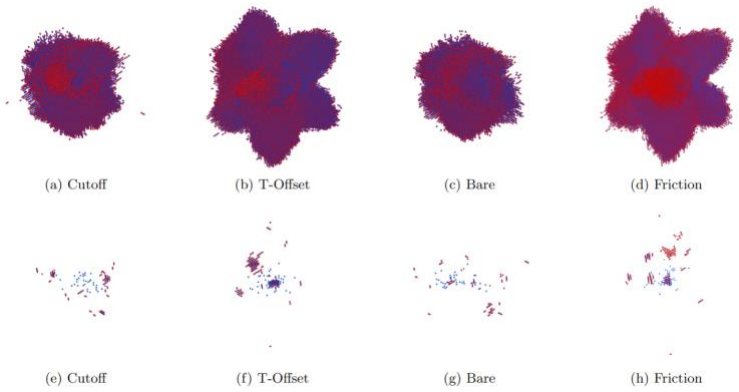

Figure 1: The damage evolution in a cascade induced by a 50 keV PKA for different treatments of electron-phonon coupling. (Top) The maximum defects count during the ballistic phase. (Bottom) The defects at the end of the cascade. The red sphere and blue squares represent the interstitials and vacancies, respectively.

Acknowledgments

This work was funded by the Leverhulme research project grand code RPG-2019-346. Via our membership of the UK's HEC Materials Chemistry Consortium, which is funded by EPSRC (EP/R029431 and EP/X035859), this work used 'ARCHER2 UK National Supercomputing Service (http://www.archer2.ac.uk). Computational resources were provided by Lancaster University's High-End Computing facility.

[1] D M Duffy, et.al., "Including the effects of electronic stopping and electron–ion interactions in radiation damage simulations", Journal of Physics: Condensed Matter, 19. 016207. (2006).