Summit to: Monte Carlo Methods and Applications

Monte Carlo Simulation of Primary Damage in Complex Materials under Ion/Neutron Irradiation

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EXTENDED ABSTRACT: Scientific understanding of any kind of radiation effects starts from the primary damage, that is, a short-range defect production and annealing process in cascades by an energetic particle. Accurate estimation of primary radiation damage is the key to understand how materials change with irradiation parameters and predict the degradation of macroscopic performance of materials. Due to the difficulties in experimental detection in the range of ~ nm and at the time-scale of ~ ps, the standard methods for studying primary damage are still the binary-collision approximation and more accurate molecular dynamics (MD) simulations [1]. In order to further break through the limitations of existing models in both accuracy and efficiency, an efficient, universal and sophisticated Monte Carlo (MC) software, IM3D, is developed for simulating primary radiation damage in arbitrarily complex materials under ion/neutron irradiation [2]. For defect production in cascades, the main advantages of IM3D are the fast indexing of scattering integrals and different stopping power database, and the choice of Constructive Solid Geometry or Finite Element Triangular Mesh method for constructing 3D shapes and microstructures [2]. For defect annealing, a concurrent cascade-annealing model is proposed in IM3D by synchronously coupling MC for cascade collisions and event-driven kinetic MC for defect evolution in the same framework [3]. The accuracy of IM3D tends to that of MD, while the efficiency is increased by at least 3 orders of magnitude. Furthermore, unlike in MD, it is not limited by interatomic potentials and defect identification algorithms. Applications of IM3D were implemented in nano-target effects in ion irradiation [2,4-6], mimicking neutron radiation effects by ions [7], electronic energy loss assessment [8,9] and cascade damage of primary knocked-on atoms [3], to reveal the general laws and new effects of primary damage in materials under ion/neutron irradiation.

Keywords： Monte Carlo; primary radiation damage; ion/neutron irradiation

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BIOGRAPHY

Prof. Yonggang Li earned his Ph.D degree at the University of Science and Technology of China in 2009 and was an visiting scholar at the Massachusetts Institute of Technology from 2012 to 2014. He was awarded as an outstanding member of the Youth Innovation Promotion Association of Chinese Academy of Sciences. He has engaged in radiation effects and defect physics of materials, by developing multiscale dynamics models including the spatial resolved arbitrarily complex structural models and high-efficient calculation methods spanning the time-scale of diffusion. His current research interests include radiation effects in nuclear materials, irradiation failure of semiconductors and multiscale computational methods. He has published more than 60 peer-reviewed papers, and been authorized 3 Chinese patents, 5 software copyrights and 1 open-source copyright.