MULTIPHYSICS SIMULATIONS OF IRRADIATION DAMAGE COLLISION CASCADES

C.P.Race*, D.R.Mason, A.P.Sutton*****

***School of Materials, University of Manchester**
****Culham Centre for Fusion Energy, Abingdon**
*****Department of Physics, Imperial College London**

ABSTRACT

Classical molecular dynamics (MD) is currently the method of choice for simulating primary irradiation damage processes. However, classical MD ignores the effect of electronic excitations on the dynamics of collision cascades. Such excitations can significantly affect the residual damage population following a cascade. Conversely, tools that are able to capture the effects of excitations, such as time-dependent density functional theory, will remain too computationally expensive for direct simulation of collision cascades for many years to come.

As a compromise, some investigators now augment the classical dynamics of their MD simulations with additional forces and degrees of freedom intended to reproduce the effect of electronic excitations on the ion dynamics. However, the models used today are mostly simple drag forces, directly opposed to the motion of the ions. These drag forces are informed by various theoretical models of electronic stopping power, but in every case the models make large simplifications (treating the electrons as a homogeneous free-electron gas, for instance).

We present the results of mixed quantum-classical simulations of collision cascades, which show that, in reality, the non-conservative forces exerted by the electrons on moving ions will be a complex tensor function dependent on the local atomic environment, the ion speed and direction of motion and the history of the electronic system. These forces are likely to have a richly varying directionality, which might well impact the residual damage caused in collision cascades. We further show that electronic excitations caused by ionic motion are manifest as an elevated electronic temperature.

We have developed a simplified classical model for the non-conservative electronic forces, which captures their rich environment dependence and yet is simple enough to be incorporated into existing large scale molecular dynamics codes at very low cost. We present

preliminary results from the use of the model to capture the effect of electronic excitations on irradiation damage.