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Atomic scale simulation in the service of nuclear materials

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Abstract content
   (Max 300 words)
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Our understanding of materials performance is based on experimental data. We use it to generate predictive models that allow us to develop improved materials and sometimes even select new materials or compositions. With nuclear energy related technologies, however, experimental data is often difficult to obtain either because the controlling factor takes place on time scales or length scales that are challenging or the hazard is such that facilities are not available. In these circumstances atomic scale computer simulations can be exceptionally useful.

We can use the results of simulation in four different ways. First, most simply, to provide property values for existing models and add context to experimental data – as we have for the potential burnable poison ZrB2. Second, to 'check' or 'test' existing assumptions such as the extent of defect volumes changes associated with fission product lattice defects. Third, to improve existing models by 'developing' the physical models – as with our understanding of the role that additives have on improving the durability of nuclear waste glass. Sometimes, however, it is possible to develop totally new models so the fourth approach uses simulations to 'discover' or 'identify' the physics/chemistry behind the process – here we will consider dislocation processes in UO2.

Thus, in this presentation we will consider these four issues in turn to illustrate how modelling and simulation adds value to the development of nuclear materials.

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