Insights into swift heavy ion induced-modification processes in a-SiO_2 and a-Ge from molecular dynamics simulations

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Molecular dynamics (MD) simulation method is an indispensable tool for understanding ion irradiation effects in materials. It is most commonly used to understand effects at the eV to keV ion energy regime but can used at the MeV to GeV regime as well when extended with the two-temperature model. Ions at this regime are called swift heavy ions ($E_{kin} \gtrapprox 1$ MeV/amu), and they can give rise to unique materials modifications along their trajectories.

We have used MD to understand two peculiar effects shown on Fig. 1: the shape transformation of gold nanoparticles (NP) embedded in a-SiO_2 and the self-organization of voids grown on a-Ge films grown on c-Ge. Both of these effects have technological relevance (for plasmonic devices and fabricating metamaterials, respectively), but their driving forces are not well understood.

In addition to the previously known role of thermal stress in the NP shape transformation [1], our simulations reveal an important contribution from adhesion between a-SiO_2 and the metal NP [2]. Current efforts are focused on understanding the role of the so-called ion hammering effects at high fluence. Similarly, in a-Ge, our simulations show that adhesion between the molten ion track and crystalline substrate plays an important role in initiating the self-organization effect. We also explore the role of ion hammering in a-Ge, which has important consequences for fundamental materials science, for example, on the question of whether a-Si and a-Ge exist as a 4-fold liquid [3].

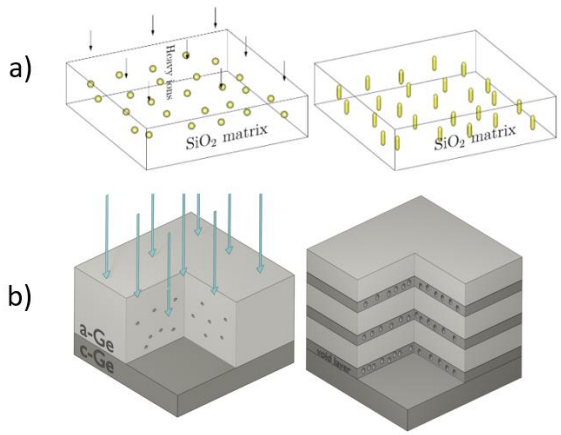

Fig. 1. Schematic presentations of the two irradiation effects a) Shape transformation of embedded Au nanoparticles in a-SiO_2 b) self-organization of voids in a-Ge

[1] C. D'Orléans *et al.*, Phy. Rev. B. **67**, 220101 (2003)
[2] A. A. Leino, V. E. Jantunen, P. Mota-Santiago, P. Kluth and Flyura Djurabekova, Sci. Rep. **13**, 6354 (2023)
[3] A. Hedler, S. L. Klaumünzer and W. Wesch, Nat. Mater **3**, 804–809 (2004)