A molecular dynamics study of irradiation creep deformation mechanisms in α-zirconium

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Abstract: Metals and alloys, such as stainless steels and zirconium alloys, used as structural materials in the nuclear core of pressurized water undergo irradiation creep deformation. The mechanical behavior is well characterized at the macroscopic level [1-4]. Yet, the underlying microscopic mechanisms are still unclear [5]. Indeed, many theoretical mechanisms have been proposed in the literature, but only few experimental results were conclusive.
Recent in situ TEM straining experiments under ion irradiation conducted on Zircaloy-4 have demonstrated that, at high stress levels, dislocations pinned on irradiation induced point defects clusters start to glide once under irradiation [6]. One of the proposed hypotheses was that the observed dislocation glide assisted by irradiation was due to a direct interaction between the displacement cascade and the pinned dislocation.
A molecular dynamics study on α-zirconium was conducted to test this hypothesis. The interaction of a screw dislocation with an interstitial loop was first studied. The objective was to pin the dislocation on the irradiation defect. The possible unpinning of the dislocation by a PKA (Primary Knock-on Atom) for stresses slightly lower than the unpinning stress was then studied. Based on these numerical simulations, a simple analytical probabilistic model was proposed to explain the irradiation creep deformation under high applied stress.

Keywords: irradiation creep, zirconium, displacement cascade, dislocations, dislocation loop.

References

[1] Gilbert, E. R., and Bates, J. F. (1977). Dependence of irradiation creep on temperature and atom displacements in 20 % cold worked type 316 stainless steel. Journal of Nuclear Materials, vol.65, pp 204-209.
[2] Fidleris V. (1988). The irradiation creep and growth phenomena. Journal of Nuclear Materials, vol. 159, pp 22-42
[3] Franklin, D.G. Lucas, G.E. Bement, A.L. (1983). Creep of zirconium alloys in reactors. ASTM STP 815
[4] Onimus, F. Béchade, J.L. (2012). Radiation effects in zirconium alloys. Comprehensive nuclear materials, vol.4, pp 1-31.
[5] Matthews J.R., Finnis M.W. (1988). Irradiation creep models - an overview. Journal of Nuclear Materials, vol. 19, pp 257-285
[6] Gaumé, M., Baldo, P., Mompiou, F., Onimus, F. (2018). In-situ observation of an irradiation creep deformation mechanism in zirconium alloys. Scripta Materialia, vol. 154, pp 87-91.