Investigation of the composite screw dislocation source activation in α-iron with irradiation defects dispersion by dislocation dynamics

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α-iron steels are widely used as structural nuclear materials, thereby subjected to radiation-induced ageing mechanisms including hardening and embrittlement [1]-[2]. These evolutions are usually ascribed to the formation of dispersed defect cluster populations, in the form of sessile dislocation loops [3]. Beyond a critical dose, plastic straining becomes heterogeneous and can give rise to defect-depleted channels, where the defect-loops are progressively removed by interaction with the mobile dislocations [4]. It is thought that channel-induced deformation can facilitate brittle fracture initiation, and is therefore regarded as a crucial damaging mechanism.

In defect-depleted shear bands indeed, mobile dislocations emitted from random sources eventually intersect a defect cluster, arresting the incoming dislocation line [5]. In this case, relatively long dislocation arms are present on both sides of the interacting defect. A screw-type arm can then change its glide plane through thermally activated cross-slip mechanism and resume gliding in its new crystallographic plane [6]. This most typical and poorly understood configuration is here called a «composite» dislocation source, which will be examined by using DD simulations (Numodis).

We investigate the movement of dislocations gliding in the presence of [1-11] and [111] sessile loops, with a view to predict interaction mechanisms and strengths representative of post-irradiation plastic straining conditions. It is found that realistic finite length sources bear significant differences with respect to the more usual, periodic boundary condition case study [7]-[8] (e.g. infinitely long dislocations, without pinning points). Namely, interaction with a [1-11] loop gives rise to the formation of a strong junction which is then by-passed by an Orowan-like mechanism. The corresponding interaction strength is then relatively high, with respect to periodic boundary conditions [8]. Interaction with a [111] loop gives rise to a helical jog that closes itself and yields the same interaction strength expression if subtracting the activation stress, with respect to periodic boundary conditions.

The case of composite screw dislocation source is investigated next. The sources include two distinct (L_{cs} , L_p) long segments, gliding in the primary and cross-slip systems, respectively. The effect of various loading conditions (τ_{cs} , τ_p) on the composite source is examined in terms of interaction mechanisms and plastic strain evolutions with time. It is observed that the dislocation arm gliding in the primary slip plane, if initially blocked by the defect, can later be liberated by the cross-slipped segment as shown in Fig. 1. The effective obstacle strength associated with this mechanism is in any case significantly lower than the interaction strength associated with the coplanar dislocation sources. Cross-slip mechanism can then greatly facilitate dislocation source activation in post-irradiated materials, depending on the local configuration and loading conditions.

Keywords: composite screw dislocation source; cross slip segment; dislocation dynamics simulation

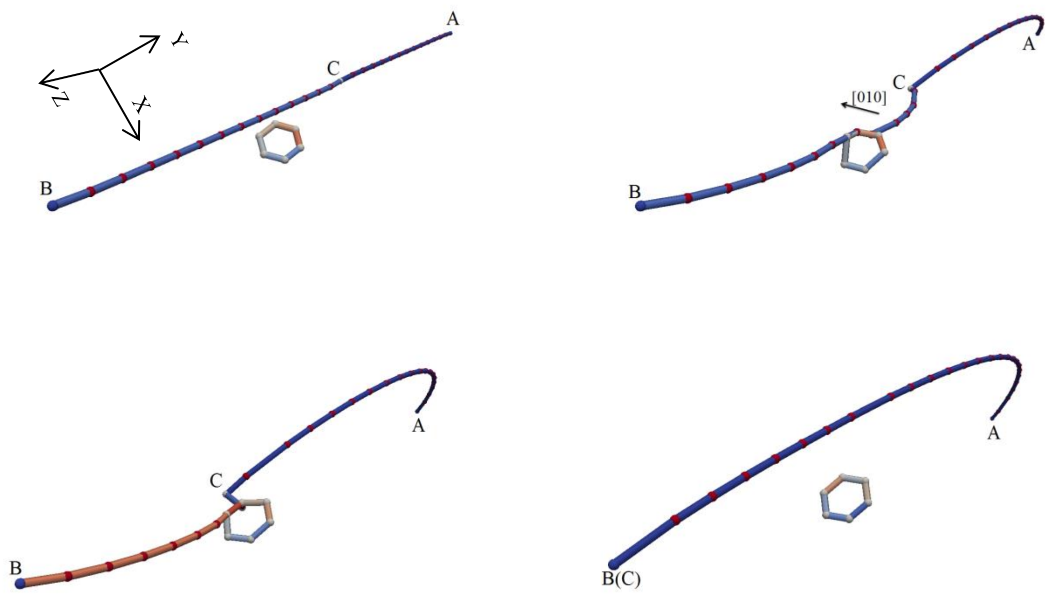

Fig. 1. Visualization of the interaction between a composite dislocation source with L_p= L_{cs}=150nm and one [1 -1 1] loop under τ_p=τ_{cs}=120MPa. The mobile screw dislocation glides in the X direction.

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