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Irradiation-induced formation of nano-crystallites with C15 Laves phase structure in bcc iron MIHAI-COSMIN MARINICA, FRANÇOIS WILLAIME, JEAN-PAUL CROCOMBETTE, CEA Saclay — The thermal diffusion of defects as vacancies or interstitials is the main process which drives the material towards equilibrium after or in parallel to the damage production. A three dimensional periodic structure is proposed for self-interstitial clusters in body-centered-cubic metals, as opposed to the conventional two dimensional loop morphology [1]. The underlying crystal structure corresponds to the C15 Laves phase. The new three dimensional structures generalize previous observations [1, 2]. By systematic exploration of the energy landscape performed using an Eigenvector Following method [3] and Density Functional Theory calculations, we demonstrate that in α–iron these C15 aggregates are highly stable and immobile and that they exhibit large antiferromagnetic moments. These clusters form directly in displacement cascades and they can grow by capturing self-interstitials. This new morphology of self-interstitial clusters thus constitutes an important element to account for when predicting the microstructural evolution of iron base materials under irradiation.

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