Stability of Vacancy Loops close to Surfaces in α-Fe from Molecular Dynamics Simulations

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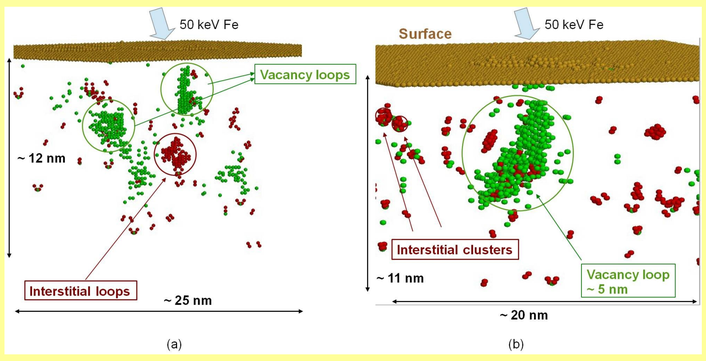
Abstract

Molecular dynamics simulations to study the stability of <100> vacancy clusters as a function of its distance and orientation with respect to the free surfaces are performed. Results show they are able to migrate to the free surfaces and recombine with it. Time for the absorption of the cluster by the free surfaces as a function of the temperature is calculated in order to obtain the migration energy activation.

Motivation

- The lack of facilities to reproduce the exact conditions in a future fusión reactor makes necessary the development of models to predict radiation materials damage or to improve material properties under irradiation.
- These models should be validated with experiments, being TEM characterization the reference technique.
- Experimental conditions (ion irradiation, thin films) are different from those for which models are developed (neutron irradiation in the bulk)
- As the main element of the reactor vessel in nuclear reactors, Fe has been largely studied for years. Nevertheless, still there are some issues as differences in the size and frequency of <100> vacancy clusters in low energy ion irradiated samples.
- Previous simulation works have shown different damage production in thin films than in bulk [1-4]. However, Molecular Dynamics still predicts higher sizes and frequencies in thin films than those observed in TEM experiments [5,6]. Differences could be due to the short time scale of the molecular dynamics simulations (on the order of tens of picoseconds) and the presence of surfaces. However, the stability of these vacancy loops has not been quantified for time scale longer than those in typical collision cascade simulations.



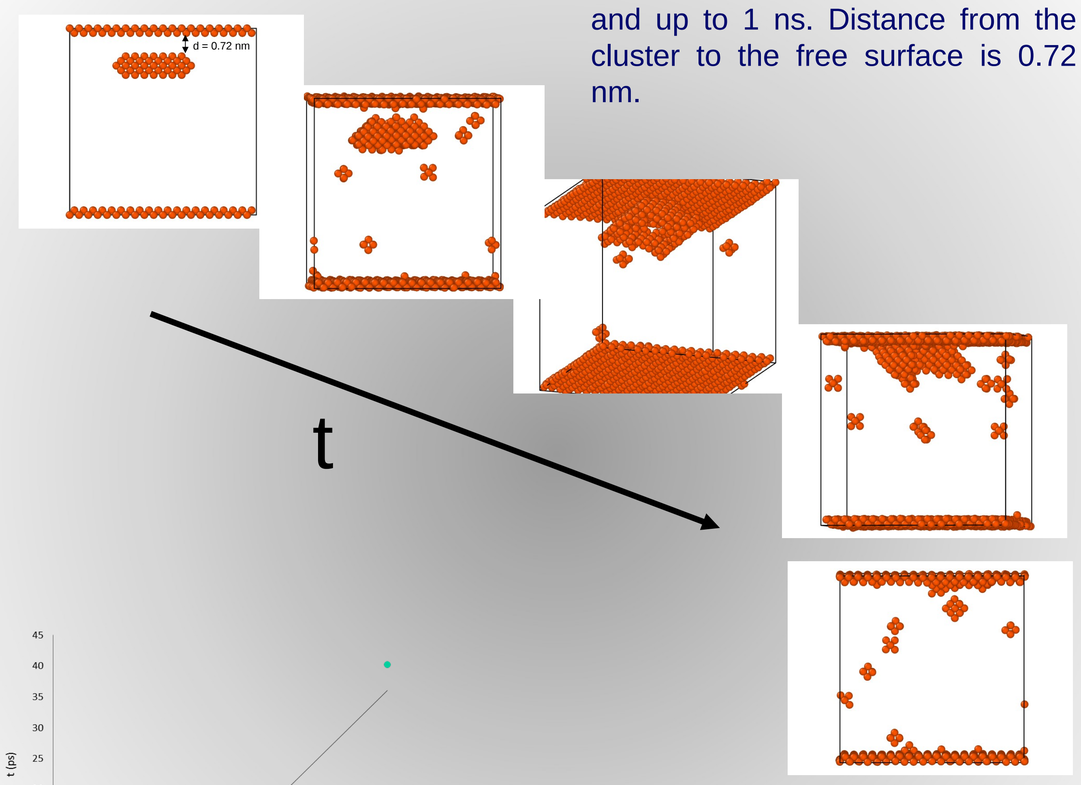
Snapshot of the Fe thin film microstructure 25 ps after launching a 50 keV Fe ion at 10º incidence angle at 0 K for two different azimuthal angles, 10º in (a) and 80º in (b) [From reference 5]

Method

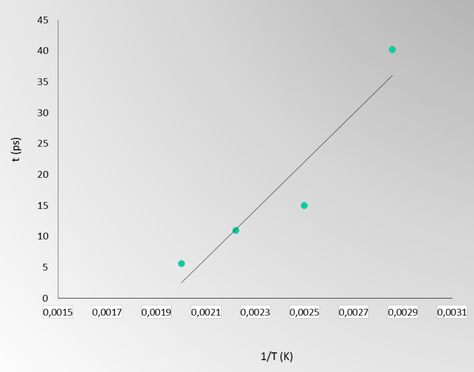
A vacancy cluster with the required orientation and distance with respect to the free surface was created and relaxed to the minimum of the potential energy. After, a Molecular Dynamics simulation is performed for a few ns, depending on the case.
Simulations were performed in bcc Fe at constant volume using the LAMMPS code [7] with the interatomic potential developed by Ackland et al. for α-Fe [8]. The analysis was performed with the OVITO [9] program and the common neighbor analysis implemented in it.
Simulation cell:
- Periodic boundary conditions along the x- and y- axes. Both surfaces along the z- direction are free.
- Volume: 20 a_0 x 20 a_0 x 20 a_0 (~ 5.7 nm^3)
- <100> vacancy clusters size: ~ 2 nm^3
- Distances cluster-free surface: 0.14, 0.72, 1.28, 1.86 and 2.47 nm
- Temperature: 300-500 K

Results: parallel vacancy clusters

T = 350 K

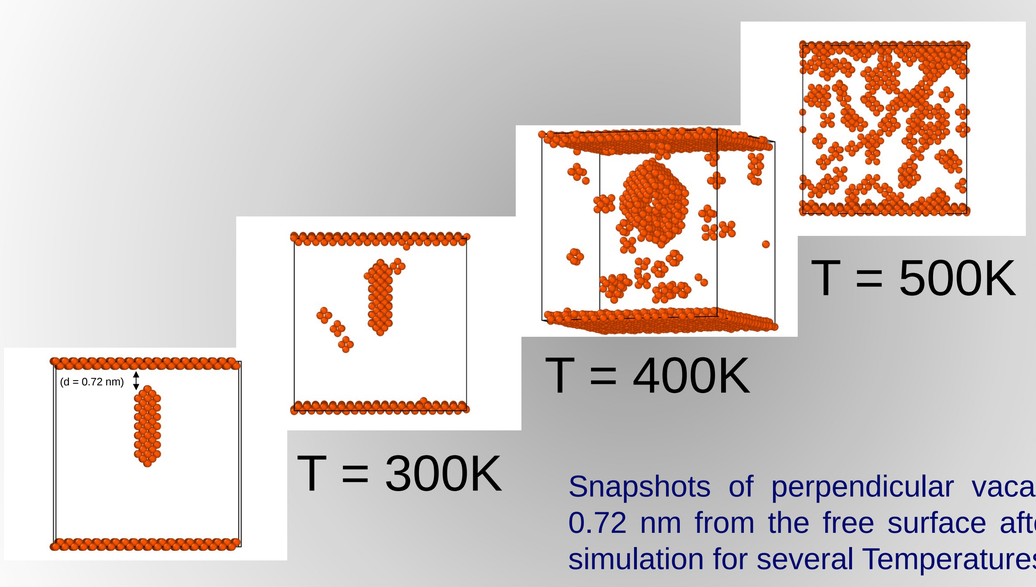


Snapshots of parallel vacancy cluster evolution in time at 350 K and up to 1 ns. Distance from the cluster to the free surface is 0.72 nm.



Snapshots of parallel vacancy cluster evolution in time at 350 K and up to 1 ns. Distance from the cluster to the free surface is 0.72 nm.

Results: perpendicular vacancy clusters



Snapshots of perpendicular vacancy cluster at 0.72 nm from the free surface after 1 ns of MD simulation for several Temperatures.

Conclusions

- <100> vacancy clusters are shown to be able to climb and disappear by recombination with free surfaces. This wouldl explain differences in the number and frequency of vacancy clusters in MD simulations with respect to TEM experiments
- Differences in the migration energy as a function of the orientation of the cluster with respect to the free surfaces are observed. Vacancy clusters oriented in parallel with free surfaces show lower migration energy
- Before the migration occurs, the cluster is reoriented

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