MD simulations of Fe precipitates in Cu

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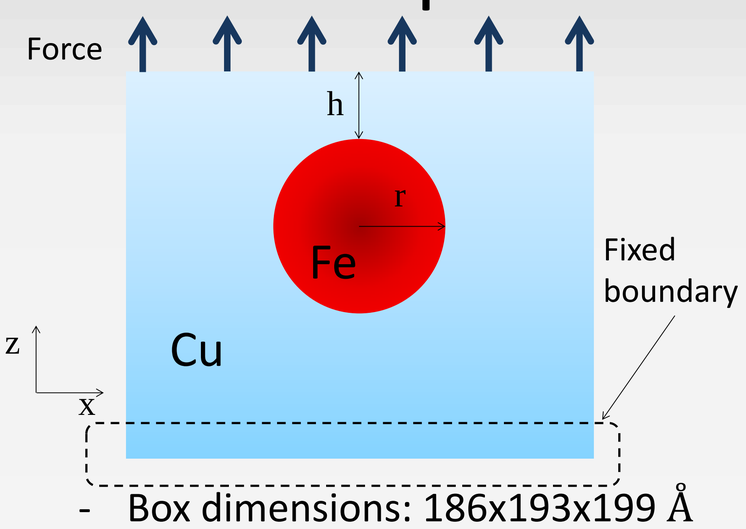
Motivation

Frequent vacuum break-downs in CLIC accelerating structures are presumably caused by field-enhancing emitters appearing on the surface [1]. The origin of these emitters is hypothesized to be caused by plastic deformations and dislocations [2]. We investigate the effect of Fe precipitates on dislocation nucleation.

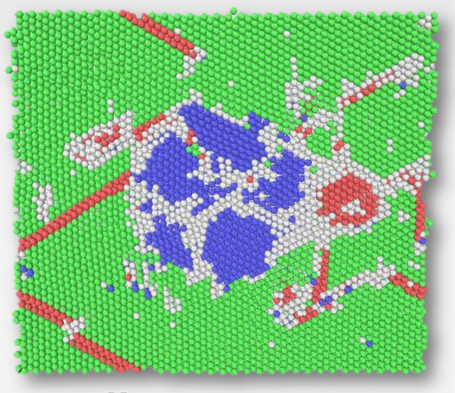
Setup



- Box dimensions: 186x193x199 Å
- Cu <110> direction in *z*
- Various *r* and *h*

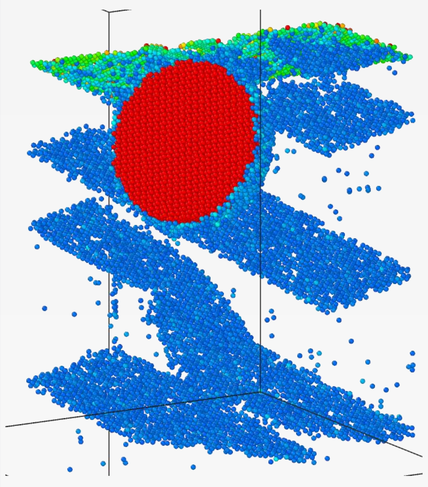
Methods

Classical molecular dynamics with LAMMPS, using the Bonny et al. many-body EAM potential. [3]



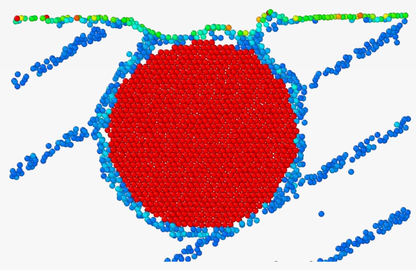
$$E = \frac{1}{2}\sum_{\substack{i,j=1 \\ j\neq i}}^{N} V_{t_i t_j}(r_{ij}) + \sum_{i=1}^{N} F_{t_i}(\rho_i)$$

Fe precipitates in Cu

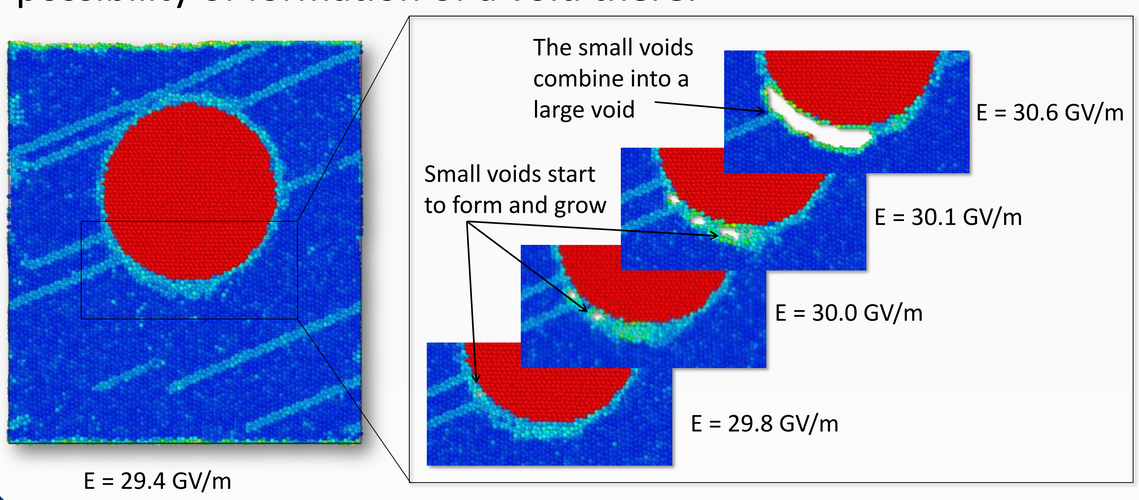

32 ps at 22.8 GV/m

Extensive stacking faults are observed in the presence of large Fe precipitates close to the surface. A depression tends to form on the surface, creating a Cu-Fe-vacuum interface and facilitating atom evaporation.

Cu atoms on a perfect lattice not shown.

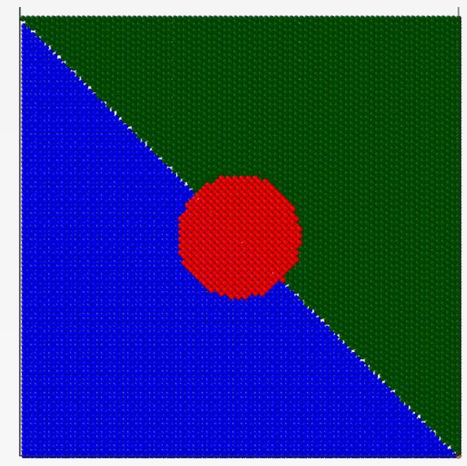

112 ps at 22.8 GV/m

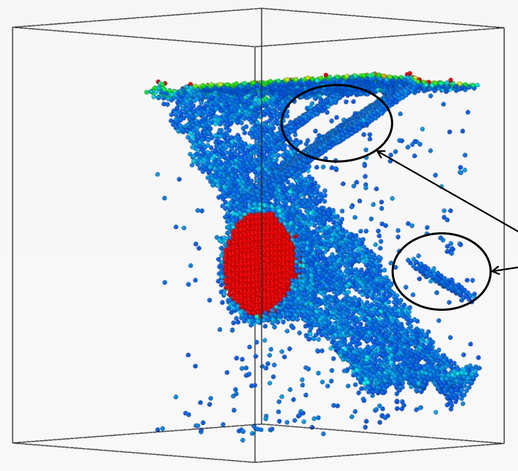
Continually ramping the electric field was found to create a void below the precipitate. The conditions correspond to a long-lasting or cyclic electric field. FEM simulations show that the stress is highest below the Fe precipitate, explaining the possibility of formation of a void there.



Grain boundary

The Fe precipitate was set on the boundary of two Cu grains, with <110> and <001> crystal directions in z. The <110> grain was exposed to the surface.



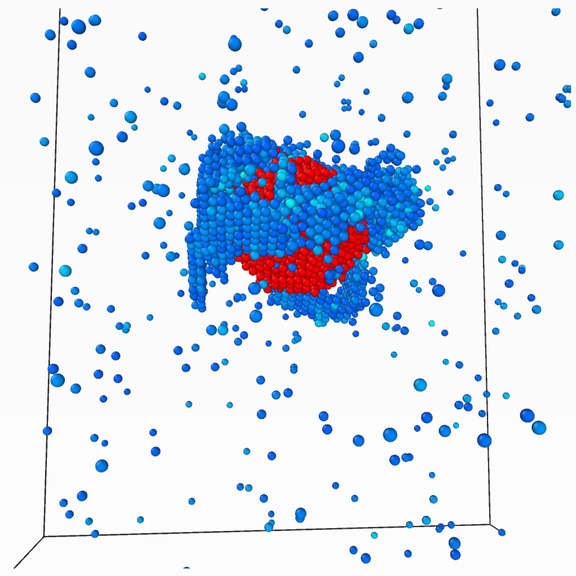

E= 25.6 GV/m

Ramping the electric field causes stacking faults to develop in two different planes. No stacking faults appear in the <001> grain. Atoms start evaporating at the surface grain boundary.

Irregular precipitates

Inserting Fe as an irregular sphere and relaxing the system causes a knot of Cu stacking faults to form around the precipitate even without an external electric field.

Cu atoms on a perfect lattice not shown.



Conclusions

- Precipitates adjacent to the surface facilitate vaporization.
- Voids can appear below the precipitate under certain conditions.
- A grain boundary may offer sites for preferential surface geometry change.
- Irregular precipitates offer more dislocation nucleation sites.

[1] Wang, J. W., Loew, G. A., *Proc Jt. Sch. Rf Eng. Accel.* (1997).
[2] Pohjonen, A. S., Djurabekova, F., Nordlund, K., Kuronen, A., Fitzgerald, S. P., *J. Appl. Phys.* **110,** 023509 (2011).
[3] Bonny, G., Pasianot, R. C., Castin, N., Malerba, L., *Philos. Mag.* **89,** 3531–3546 (2009).

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