

Molecular dynamics simulations of martensitic transformation in iron

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Propositions

Belonging to the PhD thesis of Xiaoqin Ou

Molecular dynamics simulations of martensitic transformations in iron

1. Growth of bcc phase starts in the areas of low potential energy at original bcc/fcc interfaces following the faulting mechanism with a martensitic character, which develops into the high-energy areas interfaces involving diffusional atomic jumps for a small fraction of the atoms. (this thesis)
2. The classical nucleation theory describes the evolution of postcritical bcc nuclei in fcc iron but not the nucleation event itself. (this thesis)
3. Solid-solid transformations in materials take place by nonclassical nucleation mechanisms, such as the “aggregation of nuclei” and “stepwise nucleation”. (this thesis)
4. New evidence shows that all stars have a twin (MNRAS, 2017). This is similar to the presence of a neighbouring cluster being beneficial for the stabilization of a subcritical cluster in the nucleation stage of solid-state phase transformations.
5. Strain or stress promotes the coalescence of neighbouring bcc grains, which have the same orientation relationship but in different variants. (this thesis)
6. Compared to experiments, molecular dynamics simulation is a more promising tool for examining and improving classical theories regarding microstructural evolution in materials.
7. The crystalline morphologies of martensite transformed from austenitic iron by molecular dynamics simulation agree well with those observed in steels by experiments. Molecular dynamics simulation can be used to direct the production of steels with better microstructures in industry.
8. A good scientific idea often arises after a short vacation.
9. Opportunities are hidden behind challenging difficulties.
10. The brain of a scientific researcher runs faster than his or her legs.

These propositions are considered opposable and defensible, and have been approved as such by the supervisors, Prof. dr. J. Sietsma and Dr. M.J. Santofimia Navarro.