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M02: Computational and experimental thermodynamics and kinetics of materials

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Simulation of shock waves in Fe and Fe-C using molecular dynamics

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Motivation and Objective

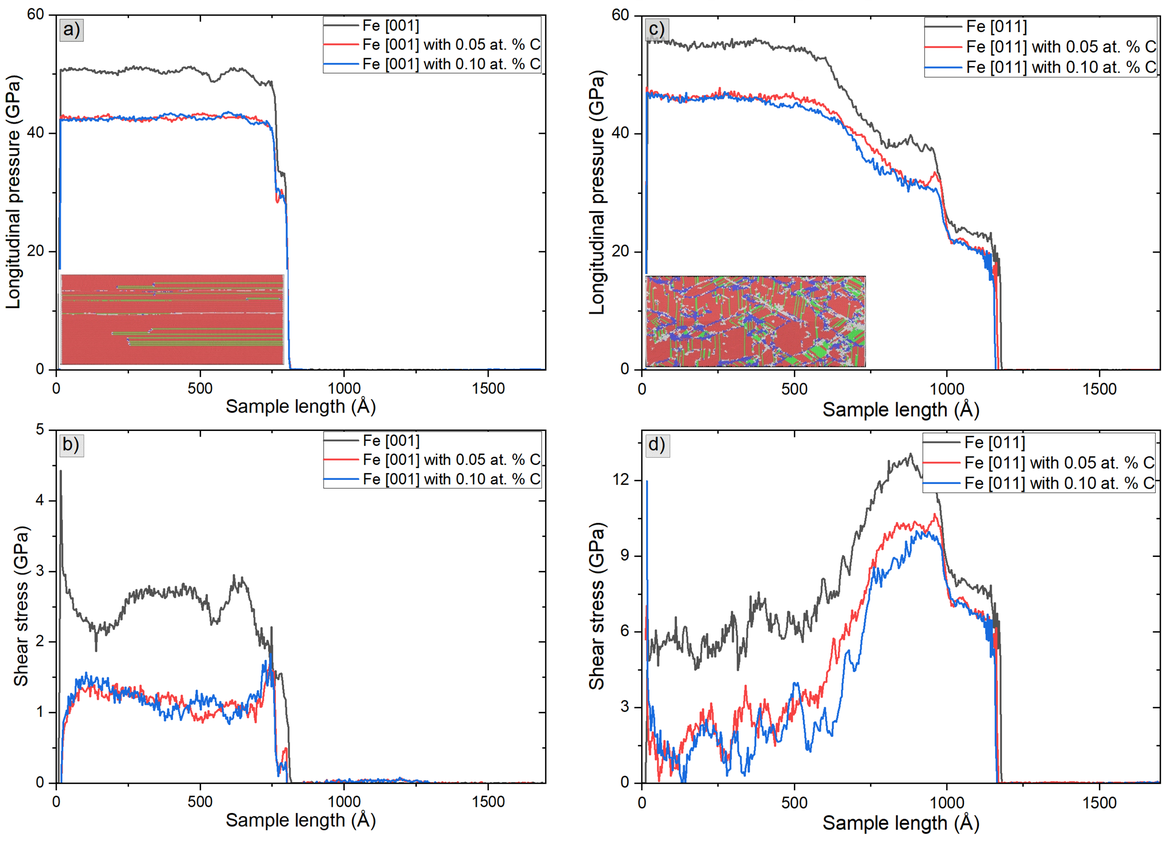
Pressure-induced phase transformation in iron and its alloys is a classic research topic in solid-state physics, material science, and geophysics. The crystal structure of iron undergoes a phase transformation at a hydrostatic pressure of 13 GPa, changing from a body-centered cubic (BCC) system to a hexagonal close-packed (HCP) system. Although extensive research has been carried out on the transformation in iron by using molecular dynamics simulations, there is very limited literature that focuses on the contribution of parent phase orientations, system size, and impurities to the phase evolution.

This study carefully examines the influence of system factors on iron and iron-carbon materials. The objective is to present an overview and to guide the community in selecting ideal settings for their simulations.

In this work, classic molecular dynamics simulations have been employed to investigate the effects of system size, lattice orientation, and impurity concentration on the pressure-induced phase transformation of iron and iron alloys for the first time.

- All simulations in this study have been done using LAMMPS.
- The interaction of iron atoms is defined by the embedded atom model interatomic potential (EAM).
- We used three simulation sets in this study to evaluate the effects of sample size on the correlation between piston velocity and shock velocity, the shock velocities and resulting phase fractions for three different shock directions, and influence of carbon on material responses.

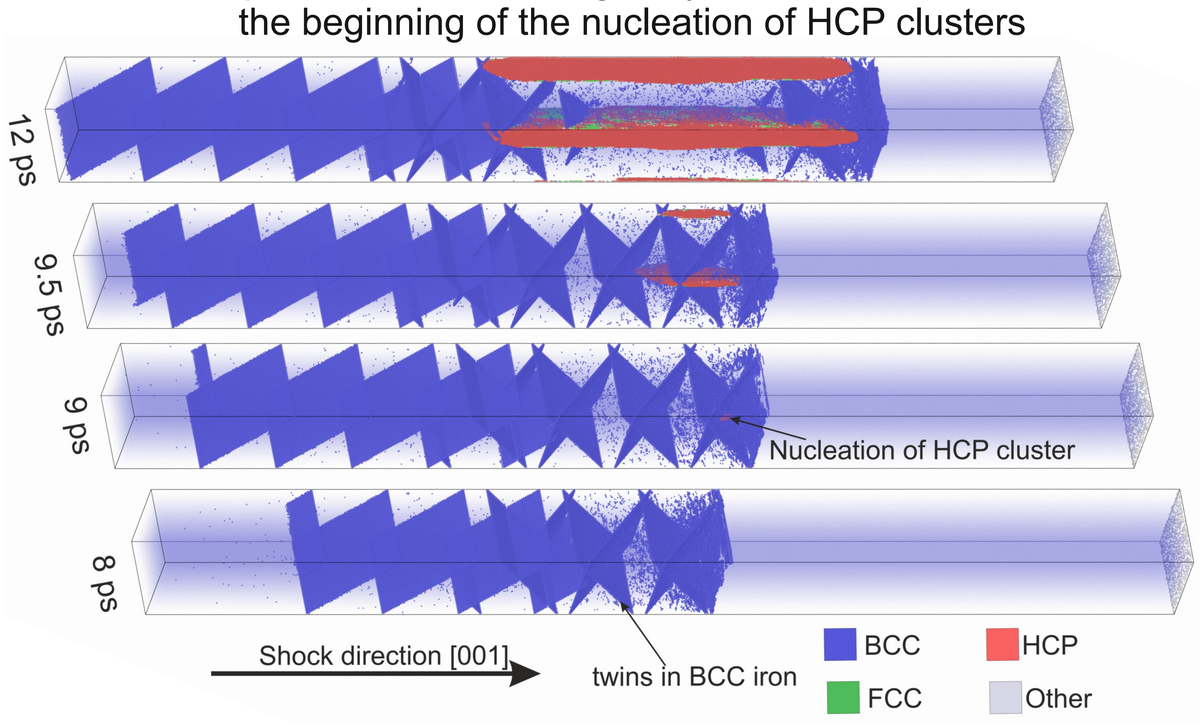
Longitudinal pressure in z-direction, and shear stress for Fe and Fe-C for [001], for [011]



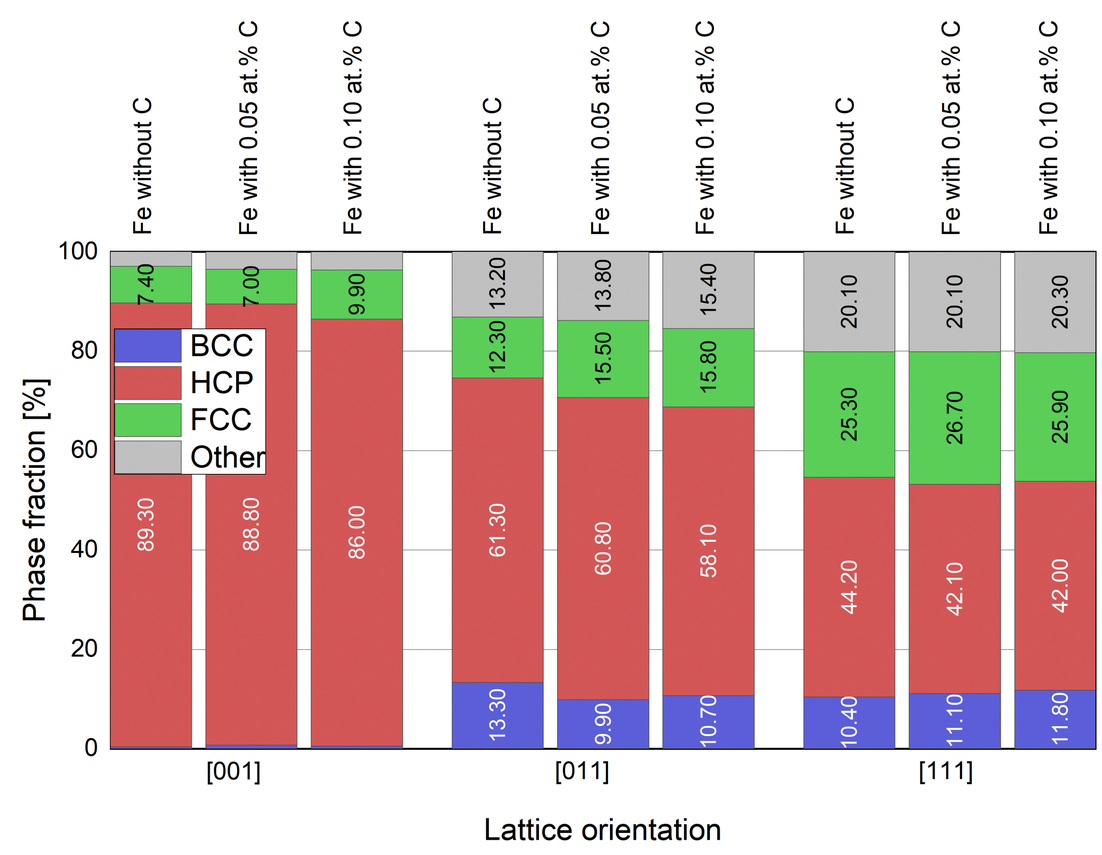
Shockwave simulations on iron and iron-carbon demonstrate that the development of the HCP phase fraction under high pressure is significantly influenced by lattice orientation. However, under dynamic compression, shock waves facilitate the material's transformation and diminish the influence of carbon instertial.

This also applies to twins when the material experiences plastic waves.

Snapshots of the iron single crystal show twins in BCC the beginning of the nucleation of HCP clusters



Phase fractions of Fe and Fe-C with 0.05% and 0.1% at. C for the lattice orientations [001], [011], and [111] for Vp0.90 km/s.



Conclusions

- The lattice orientation and carbon content both influence our shock waves in significant and different ways. The structure of the shock fronts changes based on their orientation.
- The addition of carbon is slowing down our shock waves, but the effect of carbon is increasing with increasing carbon content. However, it has little effect on the formation phase fraction of the HCP phase.
- The generated defects are different depending on the orientation. [001] shows twinning, [011] shows twinning + stacking faults, and [111] shows twinning but a higher amount of stacking faults and FCC clusters.

Acknowledgements

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