Atomistic Simulations of Ferrite and α-Fe

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Introduction

- Motivation: Most MD simulations involving ferrite (the solid solution of carbon in BCC iron) reported in the literature are carried out on pure iron.
- Probable reasons: Influence of C in ferrite is neglected maybe due to its low carbon content (0.008 % in weight).
- Carbon atoms strengthen the Fe lattice by creating strain fields and restricting dislocation movement.
- This work: Tensile test simulations of ferrite and α-Fe were carried out on the [111] direction at 300, 500 and 700 K.
- Fast strain rates: Strain rates applied were high (10^7–10^{10} s^{-1}) due to MD time scale limitations.
- **The aim is to compare the tensile properties of ferrite and α-Fe at different strain rates and to estimate the influence of carbon atoms on the mechanical behaviour of ferrite.**

Building Geometry

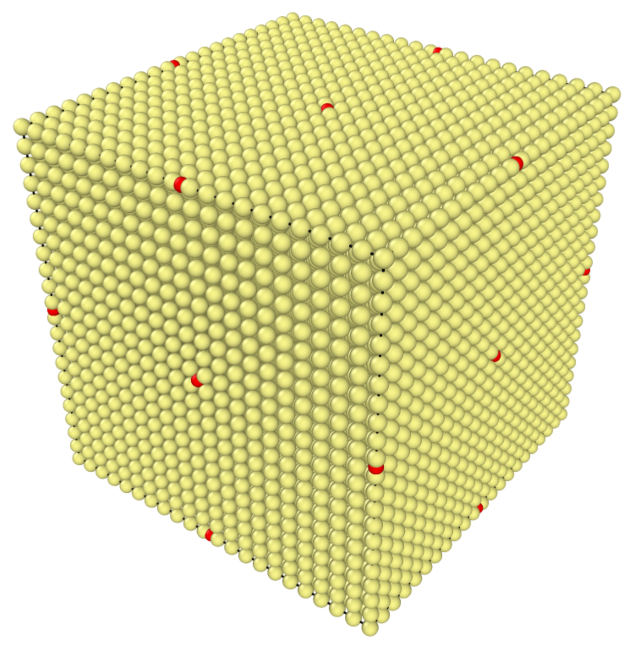


Fig. 1: Ferrite unit cell, Space group Im-3m. Carbon atoms (red) occupy octahedral sites in ferrite (Wyckoff position 6b [2]).

Simulation Set Up

Parameter	Set Up
Number of atoms	2.3×10^6
Dimensions	300 x 300 x 300 Å^3
Interatomic potential	Hepburn and Ackland [1]
Integration timestep	1 fs
Boundary conditions	ppp

Table 1: Parameters used in the simulations. p: periodic boundary conditions.

Equilibration

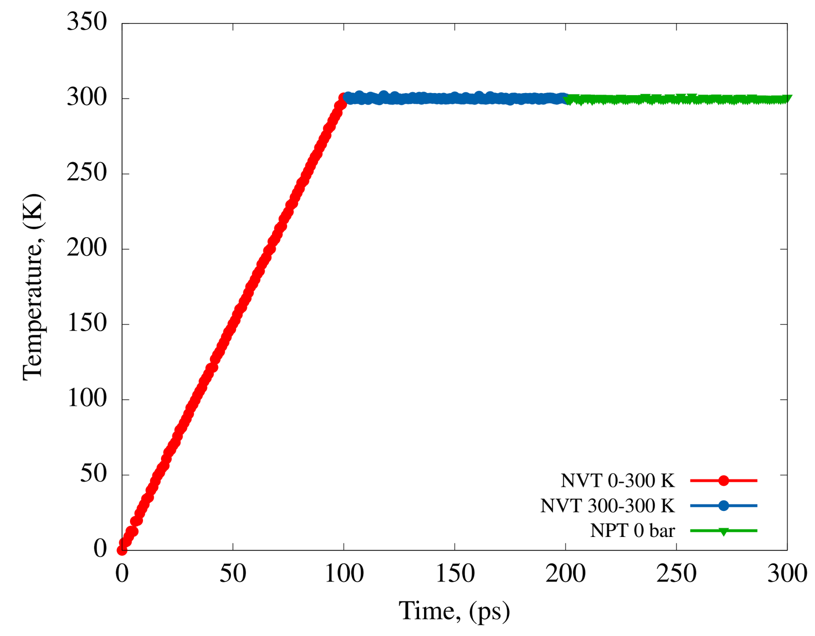
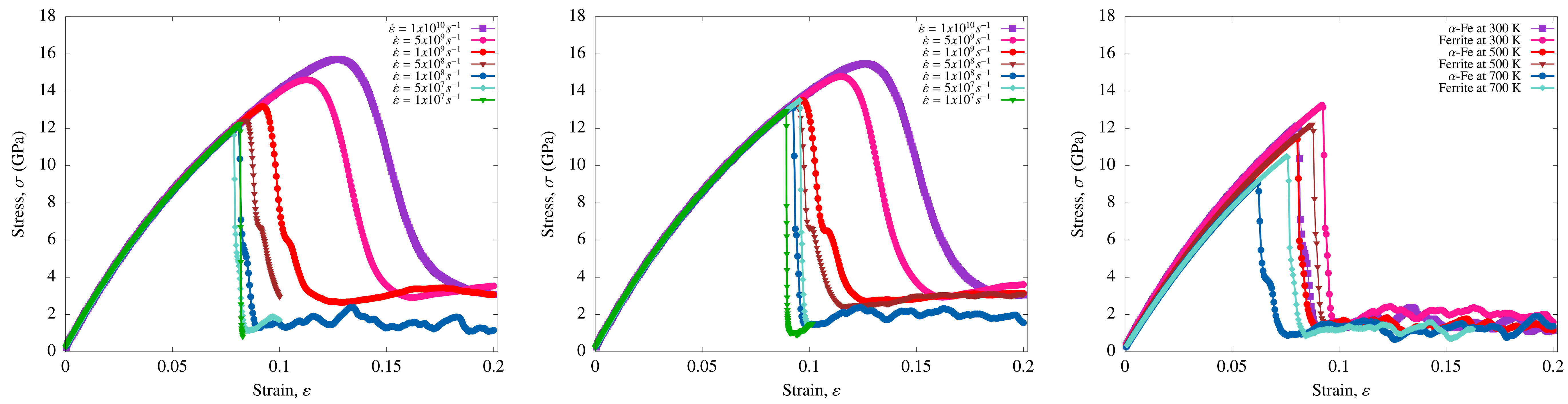


Fig. 2: Temperature versus time and ensembles used during equilibration.

Tensile Test Simulations



(a) α-Fe (b) Ferrite (c) α-Fe and Ferrite at $\dot{\varepsilon} = 10^8\,s^{-1}$

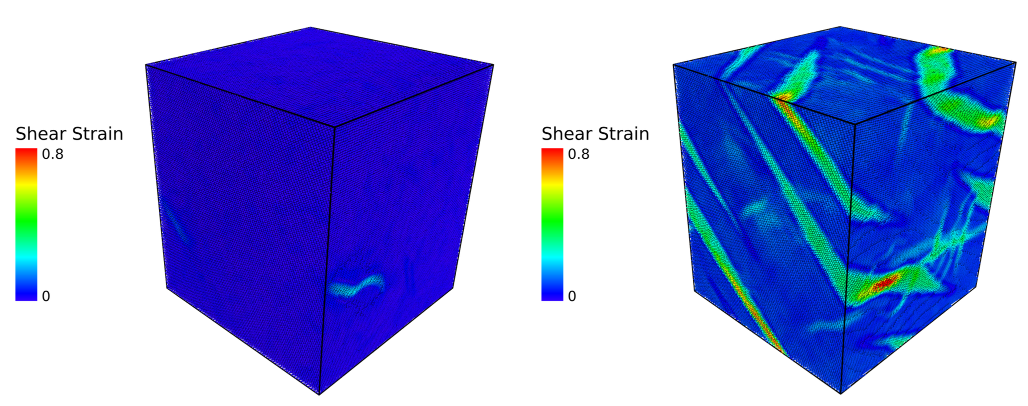
Fig. 3: Stress-strain curves showing that the difference in mechanical behaviour between α-Fe and ferrite become more significant at lower strain rates and higher temperatures.

Strain Rate Sensitivity

Table 2: The strain rate and yield strength relationship is described by $\sigma_y = C\dot{\varepsilon}^m$.

	Temperature	m	C (GPa)	$\sigma_{\dot{\varepsilon}=10^{-3}s^{-1}}$ (GPa)
α-Fe	300 K	0.035	6.86	5.40
	500 K	0.049	4.70	3.34
	700 K	0.069	2.70	1.67
Ferrite	300 K	0.022	9.34	8.02
	500 K	0.030	7.42	6.01
	700 K	0.037	5.69	4.39

Deformation Mechanism



(a) $\varepsilon = 0.09$ (b) $\varepsilon = 0.1$

Fig. 4: Deformation process of Ferrite at 700 K. (a) Dislocation nucleation. (b) Dislocation propagation and activation of secondary slip planes.

Stresses and Slip Planes

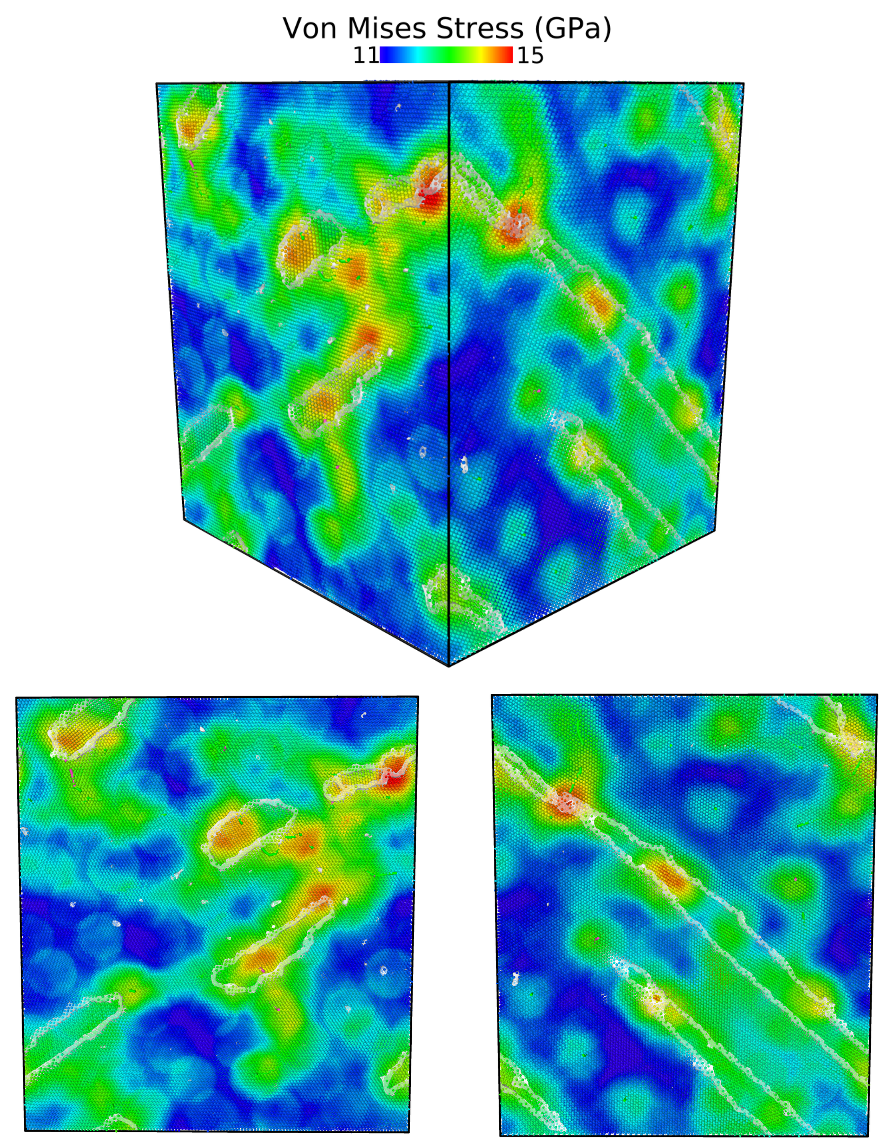


Fig. 5: Typical stress map after yield. Regions of higher stress are located along slip planes and dislocation junctions. The stress field acting on C atoms can also be visualised.

Carbon Diffusion

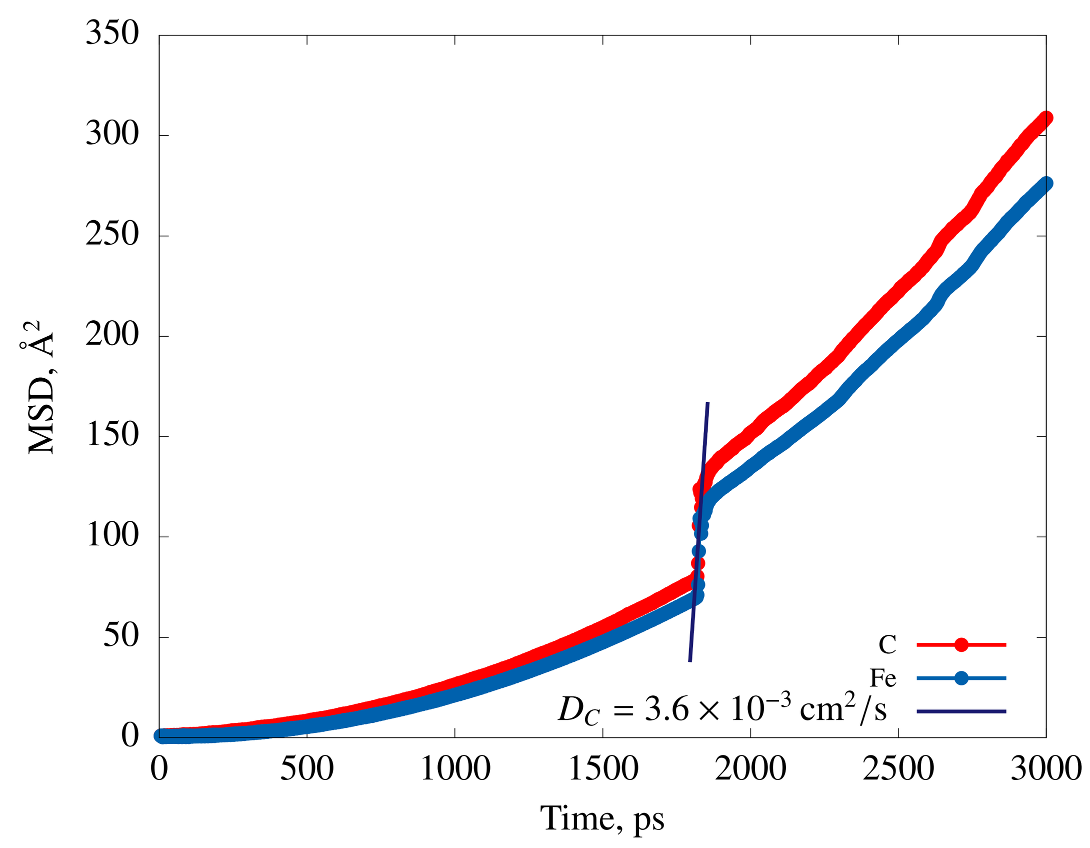


Fig. 6: Mean square displacement of C and Fe versus time. During the deformation process, three stages can be identified: an elastically dominated region, yielding and a plastically dominated region.

Conclusions

- An important difference between the mechanical behavior of pure iron and ferrite indicates that using only Fe atoms to represent ferrite will result in errors.
- The strain rate sensitivity of the yield strength is described by $\sigma_y = C\dot{\varepsilon}^m$, with higher m values for α-Fe than for ferrite.
- The value D_C during yield was calculated as $3.6 \times 10^{-3}\,\text{cm}^2/\text{s}$.

References

[1] Hepburn, D. J. and Ackland, G. J *Phys. Rev. B*. 2008, 78, 165115
[2] Bhadeshia, H. K. D. H. *Journal of Materials Science*. 2004, 39, 3949–3955

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