Atomistic simulations of the shock and spall behavior of the refractory high-entropy alloy HfNbTaTiZr

SWZ-Mini-Workshop „Simulation meets AI“

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Table of Contents

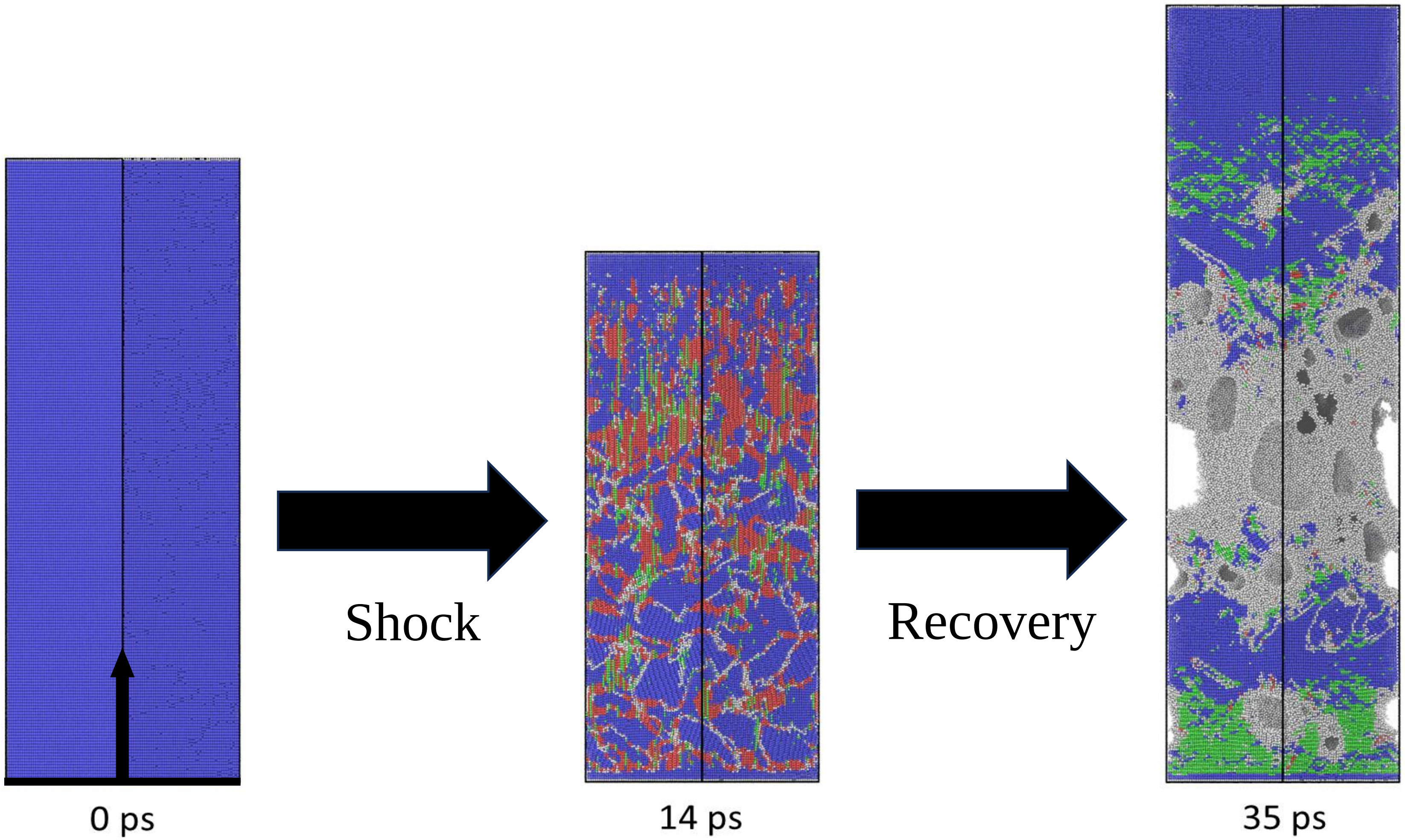
1. Introduction

- High-entropy alloys (HEA) are getting more attention because of their promising mechanical properties
  - Good ductility, corrosion resistance, and high yield strength
- Material of interest is the quinary equiatomic HfNbTaTiZr known as the Senkov alloy
- Experimental work only exists for low strain rates
- Studied the effect of shock wave on the refractory HEA
- Investigated are shock propagation and spall, phase transformation and twinning, dislocation plasticity, and spall strength

2. Methods

- Embedded-atom-method-type potential by Xu et al. [1] used to model HfNbTaTiZr alloy
- Single crystal bcc sample created
  - ~ 1.2 million atoms
  - Lattice constant of a_0=0.3404 nm
  - Periodic boundary conditions in x and y direction, non-periodic in z direction
  - ~ 18.5 nm x 18.5 nm x 72.2 nm
- Two different minimization styles are used: FIRE and conjugate gradients
- Temperature rescale algorithm applied:
  - Heating up to 700 K in 20 ps
  - Held for 100 ps
  - Cooled down to 0 K over 100 ps

2. Methods



2. Methods

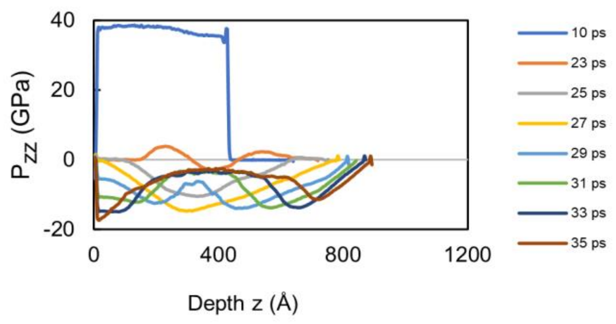
- Three different piston velocities are used: 0.8 km/s, 1.2 km/s, 1.6 km/s
- Two elements of the stress tensor are particularly relevant:
  - P_{zz}, the normal stress in z direction
  - $\tau_{\ shear}$, the shear stress which is calculated as followed:

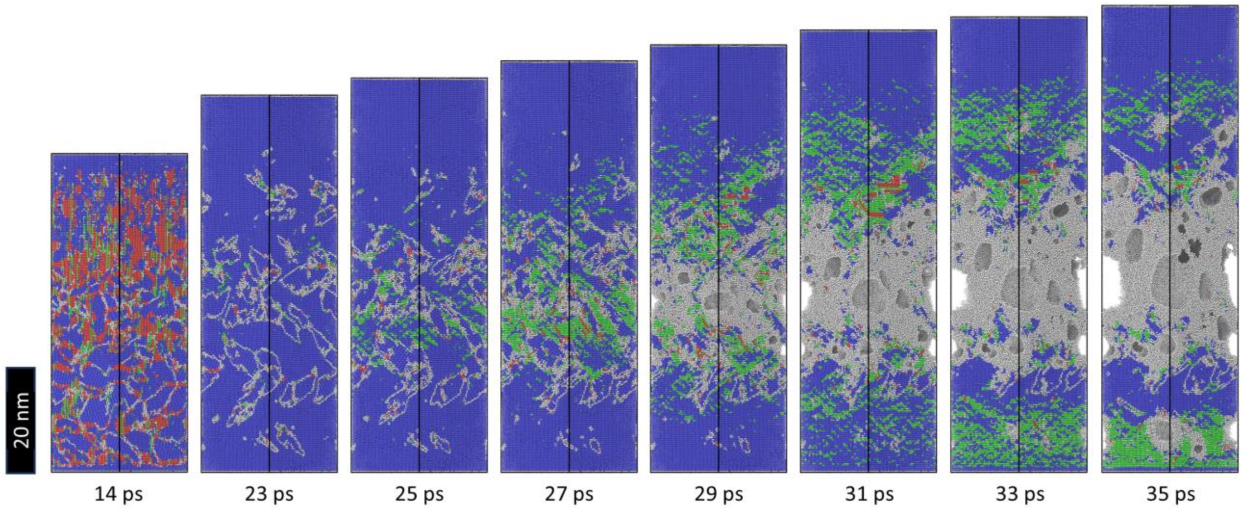
$$\tau_{shear} = \frac{1}{2}(\sigma_{zz} - \frac{\sigma_{xx} + \sigma_{yy}}{2})$$

- Polyhedral Template Matching (PTM) with a Root-Mean-Square Deviation (RMSD) value of 0.1 used to identify the microstructure in OVITO

3.1. Shock propagation and spall

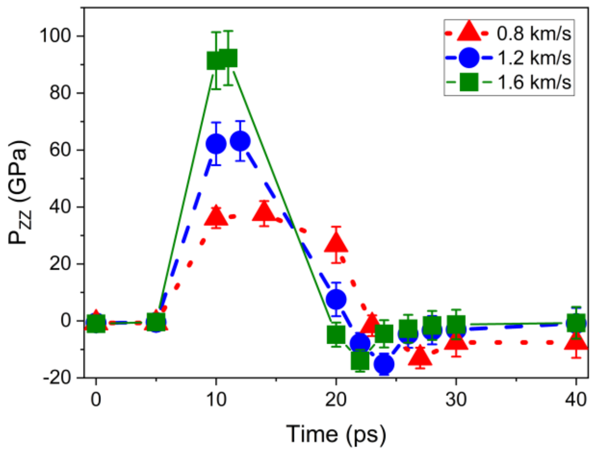
- Shock waves getting reflected at free surface → overlap creates a tensile pulse
- Spallation starts in the middle of the sample
  - Series of tiny voids created and amorphization occurs
  - Stronger shock waves → many cracks + spall at multiple nucleation sites
  - Weakest shock wave → spall concentrated in the middle

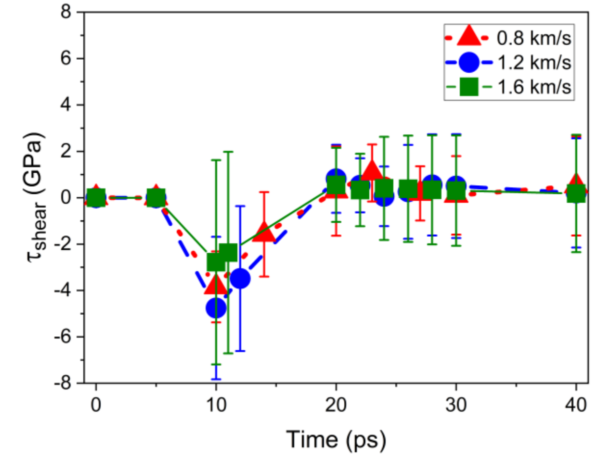




3.1. Shock propagation and spall

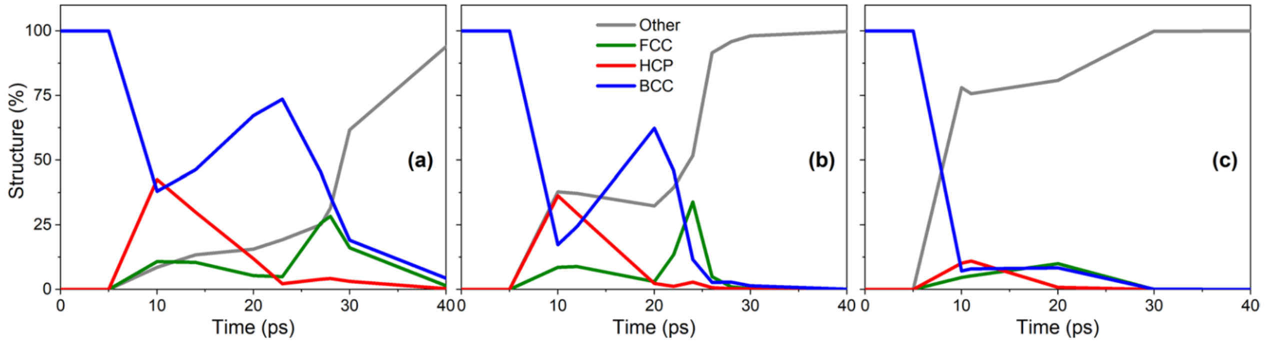
- Temporal evolution of two important stress characteristics
  - Stress along z direction, P_{zz}
  - Shear stress, $\tau_{\ shear}$
- Error bars increase with increasing shock velocity and are caused by pressure fluctuations
- Temperature increase during spall is large, small during shock
  - Almost reaching melting point during spall



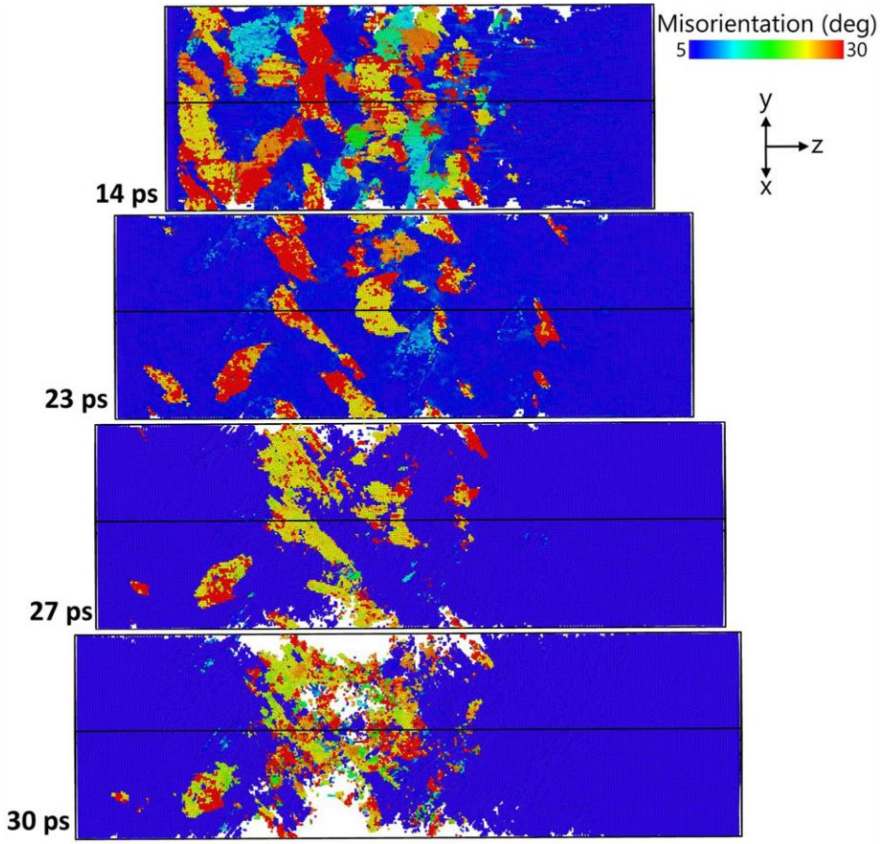


3.2. Phase transformation and twinning

- Phase transformation the moment shock reaches bcc structure
  - Forms close-packed phase; hcp and fcc, hcp dominating
- Increase in shock strength ➡ decrease in bcc-%, increase in other-%
  - Other = unidentified structure
- Why? ➡ high shear pressures ➡ destroy periodic crystalline structural environments



3.2. Phase transformation and twinning

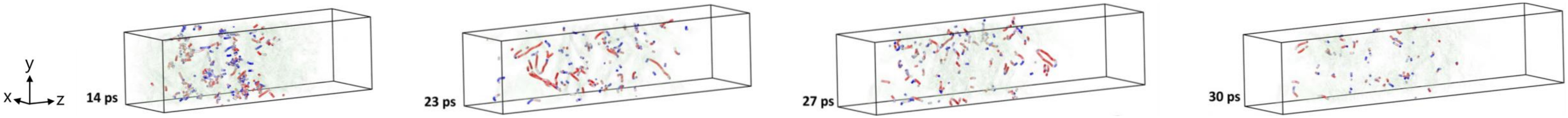


- Shock compression causing massive amounts of twinning in the sample
  - Reflection at free surface leads to reduction of twinning ➡ Reason? ➡ Tensile pressure
  - Spall shatters twins

- Large number of twins in agreement with refractory HEA VNbTaTiZr study [2]
  - Primary deformation is through twinning

3.3. Dislocation Plasticity

- Dislocation activity
  - Increasing with increasing time
  - Decreasing with increasing shock strength
  - Reflection leads to decrease in total dislocation length
- Short dislocation segments
  - Created by the twinning process within nanocrystalline structure
- Screw-type dominate edge-type dislocation
  - Plasticity dominated by gliding of screw dislocations [3-5]



3.4. Spall strength

- Obtained using formula on the right [6]
  - Mass density = 10 g/cm³, sound velocity = 3.9 km/s from elastic constant C_{11}
- Atomic stresses more reliable than calculation using back-surface velocity profiles
  - Equation using approximations of wave propagation in a solid

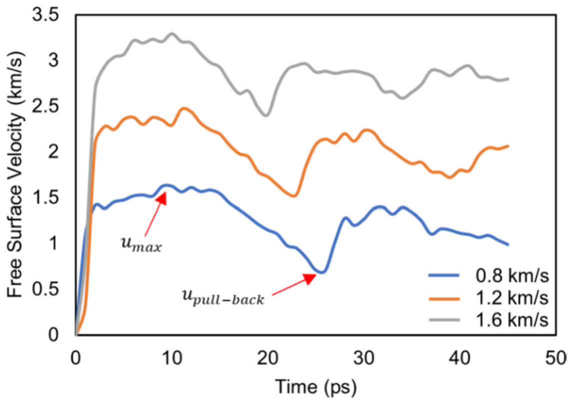
$$\sigma_{spall} = \frac{1}{2}\rho_0 c_0 \Delta u$$

Initial density

Bulk sound velocity

$$\Delta u = u_{max} - u_{pull-back}$$

U_p (km/s)	σ_{spall} (GPa)	P_{zz} (GPa)
0.8	17.9	14.9
1.2	18.2	15.4
1.6	17.3	14.1



4. Summary

- Twinning = important mechanism, especially for smaller piston velocities
- Phase transformation essential for establishing twin structure
- Bcc transforming into hcp + fcc
- Dislocation plasticity rather less important
  - Mostly short segments, long segments rare
- Screw-type dislocations dominating after shock compression

Sources

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