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

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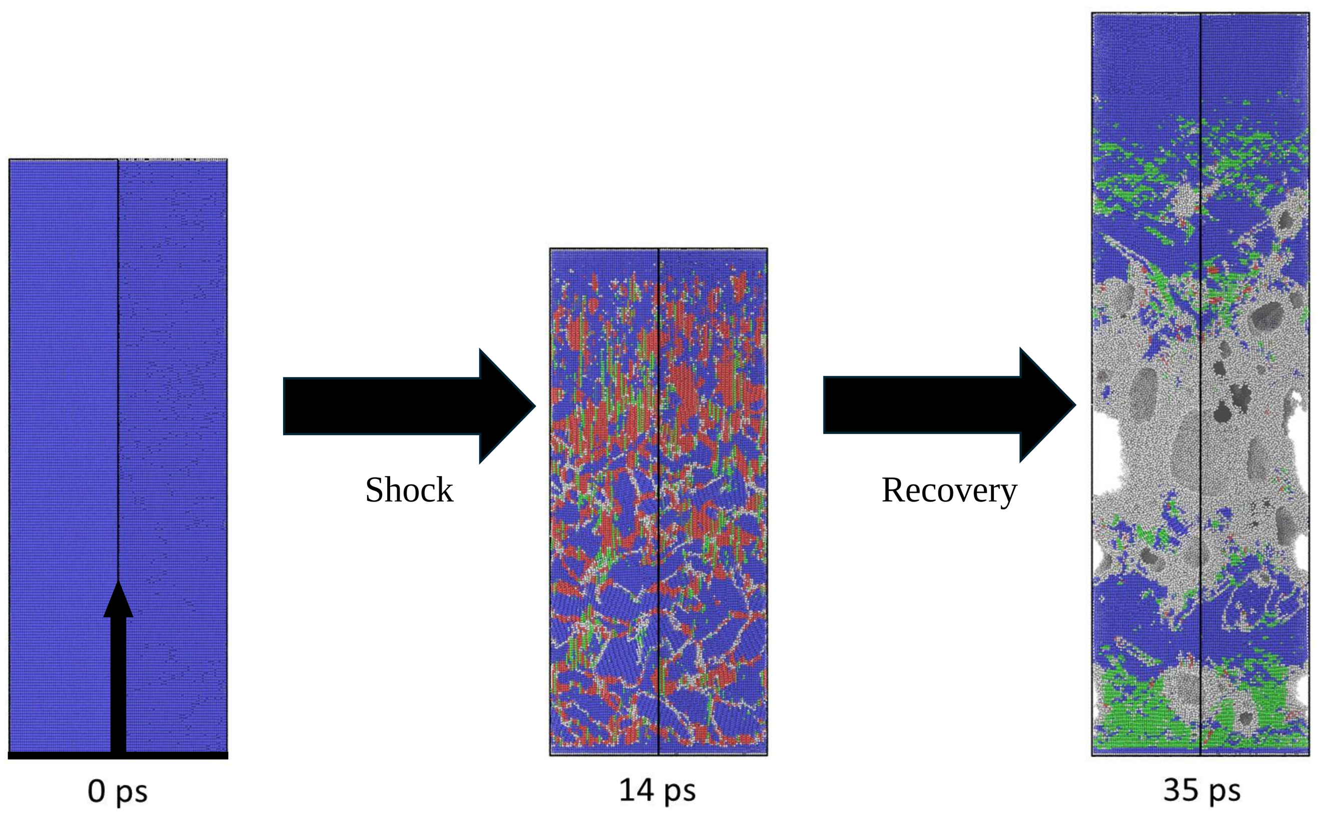
Motivation:

High-entropy alloys show promising mechanical properties, such as good ductility, corrosion resistance, and high yield strength. The connection between microstructures and compositions with their properties is already extensively investigated for compression [1, 2], tension [3], and indentation [4], but their high-pressure properties aren't. To advance our understanding, we studied the Senkov alloy (HfNbTaTiZr) under shock compression in LAMMPS.

Dislocation Plasticity:

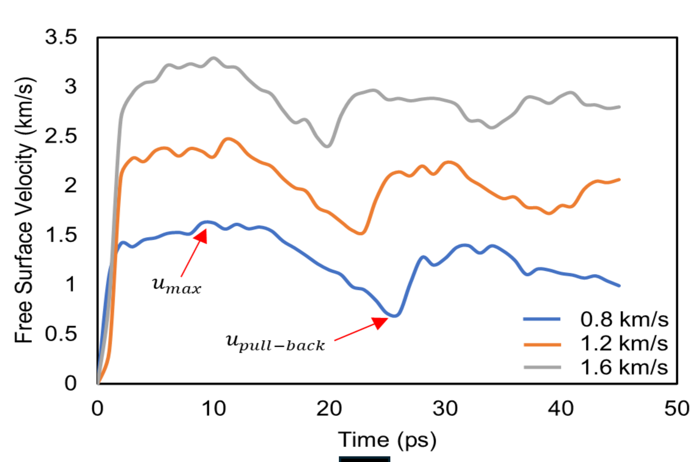
The embedded-atom-type potential developed by Xu [5] is utilized to simulate a single crystal of HfNbTaTiZr with a lattice constant of a_0 = 0.3404 nm. A layer of atoms serves as the piston, accelerating along the z-direction at three different velocities: 0.8 km/s, 1.2 km/s, and 1.6 km/s. The single crystal undergoes shock until the shock waves reach the free surface. A corresponding dump file, recorded shortly before impact, marks the start of the recovery simulation. OVITO is employed to investigate the spall and microstructure, with the latter being analyzed using Polyhedral Template Matching.

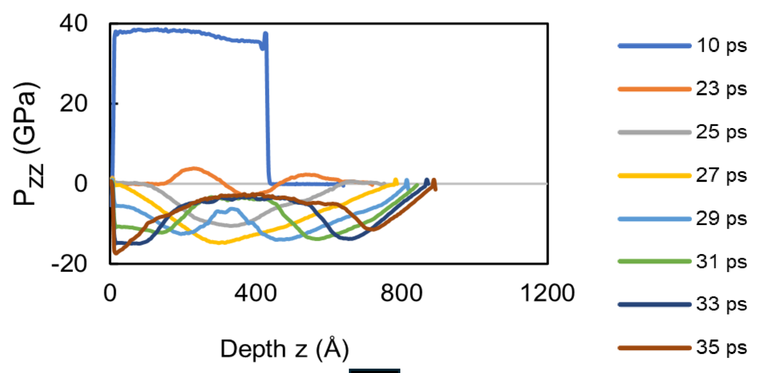
Simulation-Process:



Simulation-process visualized using snapshots from shock- and recovery simulations. The arrow shows the travel direction of the shock wave. The black lines indicate the simulation volume, and the shock moves from bottom to top.

Spall Strength:

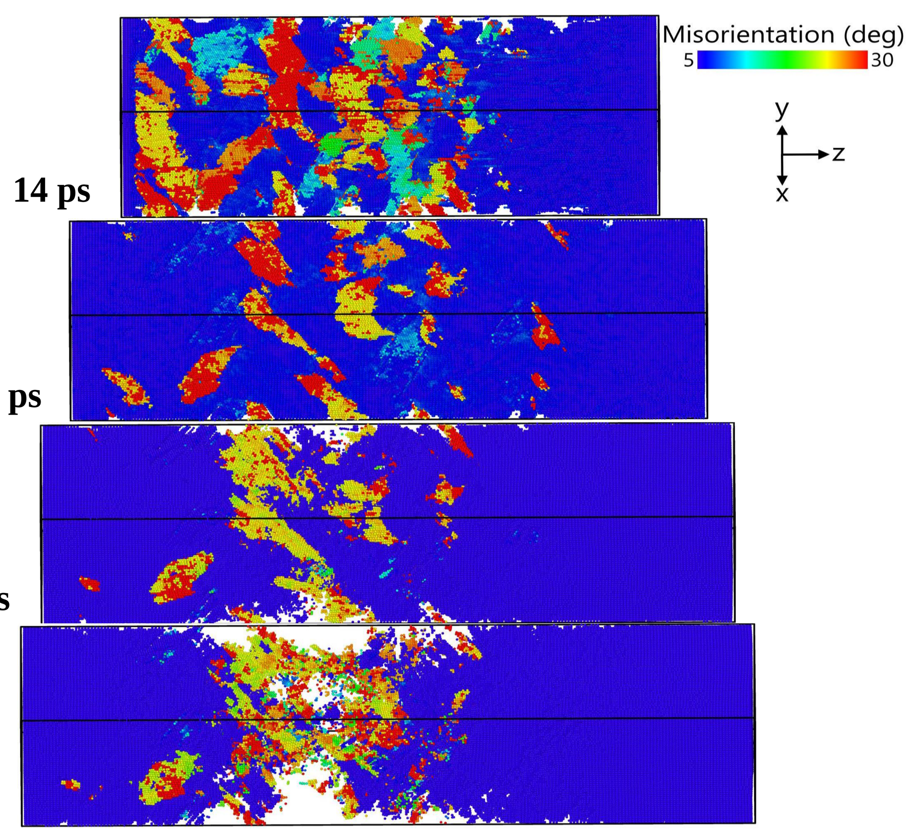




$$\sigma_{spall} = \frac{1}{2}\rho_0 c_0 \Delta u$$

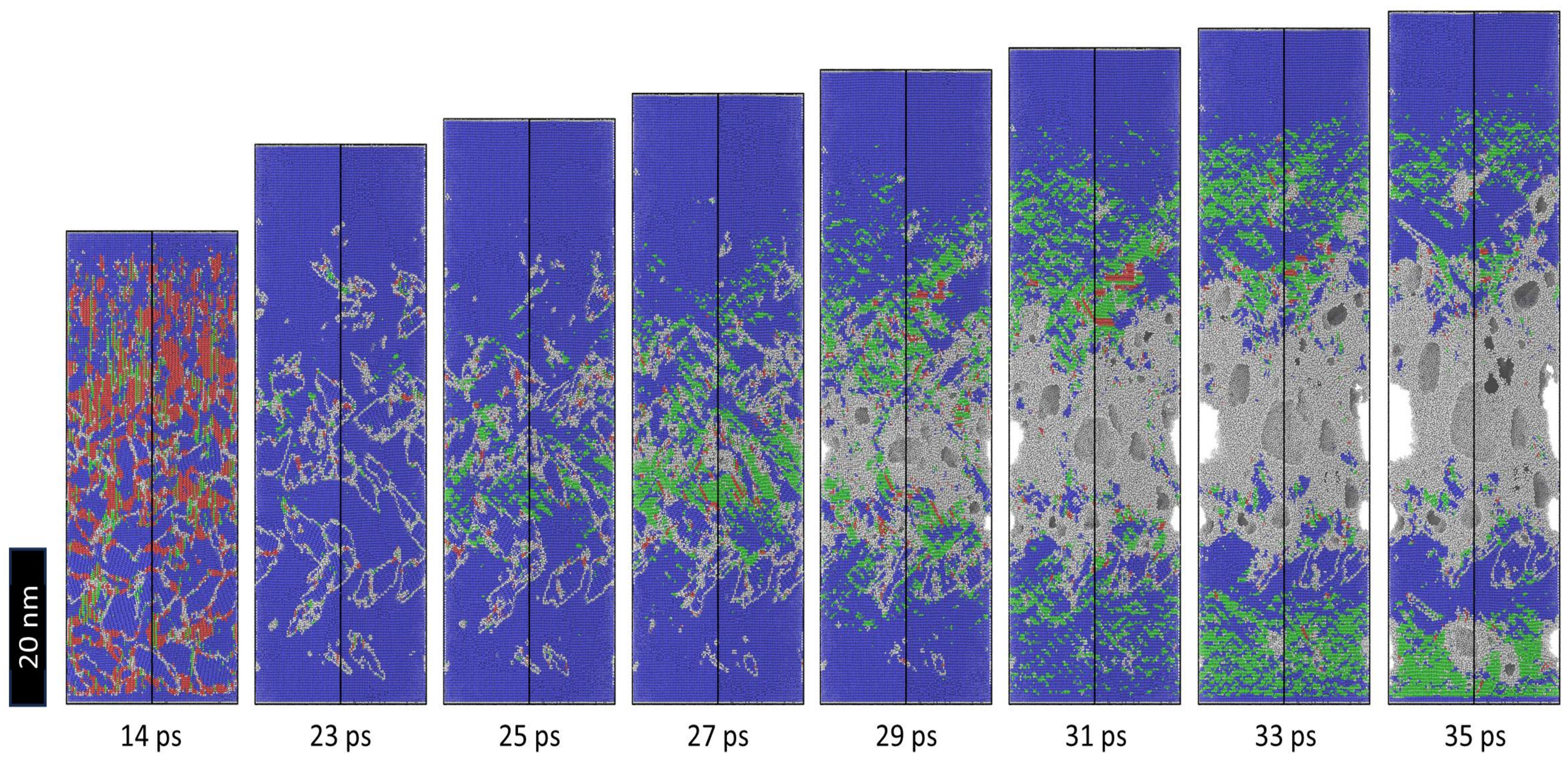
$U_P\ (\frac{km}{s})$	$\sigma_{spall}\ (GPa)$	$P_{zz}\ (GPa)$
0.8	17.9	14.9
1.2	18.2	15.4
1.6	17.3	14.1

Twin Development:



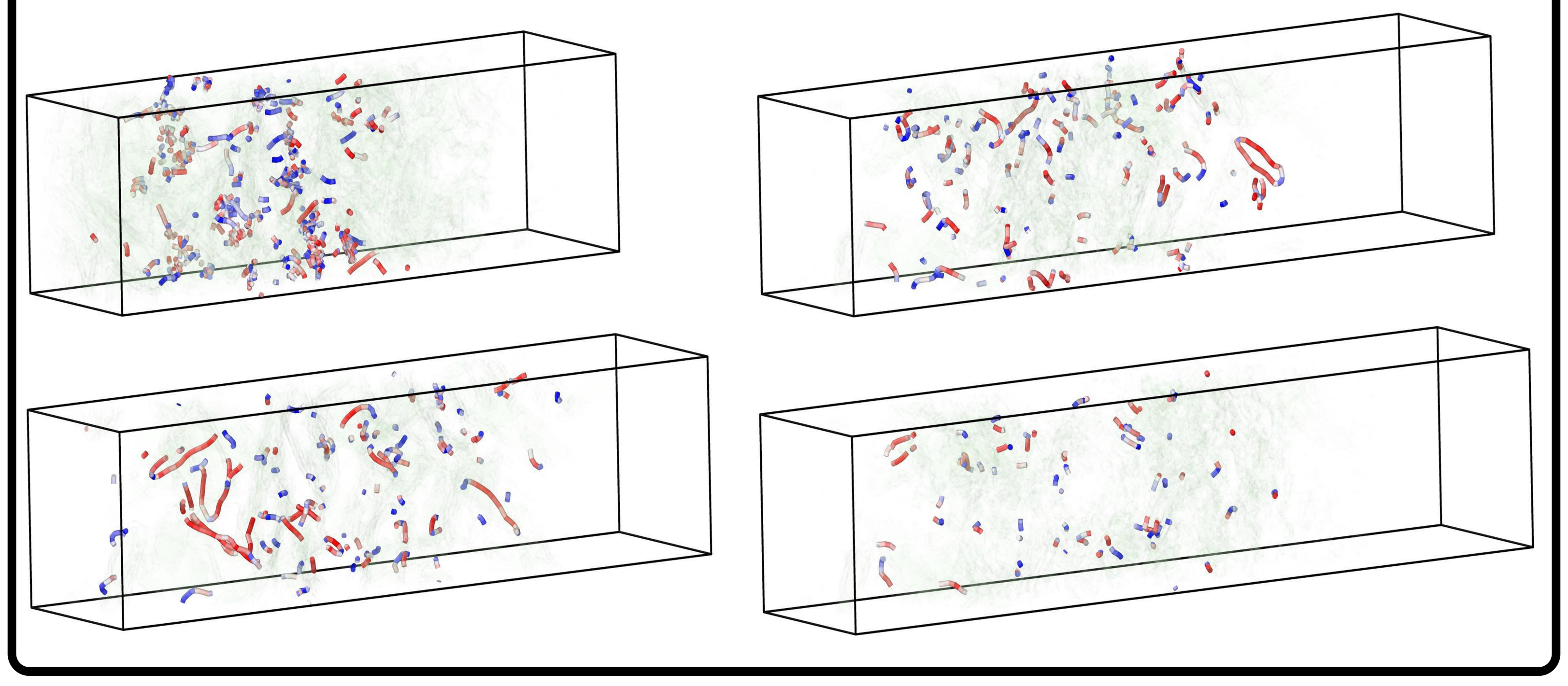
Snapshots on the left show the twin variants development colored in the bcc phase using 0.8 km/s piston velocity. The misorientation angle is set in comparison to the original bcc variant.

Phase Transformation:



PTM is used to colorize the microstructure locally during spall. The colors are as follows: red (hcp), blue (bcc), green (fcc), and light grey (other).

Dislocation Plasticity:



Summary:

1. Twinning is an important plasticity mechanism, in particular for the smaller piston velocities.
2. Phase transformations play an essential role in setting up the twin structure.
3. The bcc phase also transforms into close-packed structures: fcc and hcp.
4. In contrast, dislocation plasticity is of minor importance. While dislocations do occur at the interfaces of twin variants, long line segments within the forming nanocrystals are rare.
5. Free dislocation segments preferentially feature screw rather than edge character in the relaxed phase after shock compression.
6. HEA complexity does not reflect increased spall resistance. The calculated values are smaller compared to Ta.

Literature:

[1] Dirras, G., et al. "Mechanical behavior and microstructure of Ti20Hf20Zr20Ta20Nb20 high-entropy alloy loaded under quasi-static and dynamic compression conditions." Materials Characterization 111 (2016): 106-113.

[2] Ren, Kerong, et al. "Dynamic compression behavior of TiZrNbV refractory high-entropy alloys upon ultrahigh strain rate loading." Journal of Materials Science & Technology 161 (2023): 201-219.

[3] Sun, Jiacheng, et al. "Tensile behavior and microstructural evolution of TiMoZrV HEAs: a molecular dynamics study." Applied Physics A 130.2 (2024): 95.

[4] Chen, Yuan, et al. "Chemical short range order and deformation mechanism of a refractory high entropy alloy HfNbTaZr under nanoindentation: An atomistic study." Journal of Materials Research and Technology 24 (2023): 3588-3598.

[5] Xu, Shuozhi, Wu-Rong Jian, and Irene J. Beyerlein. "Ideal simple shear strengths of two HfNbTaTi-based quinary refractory multi-principal element alloys." APL Materials 10.11 (2022).

Additional Information:

Scan this QR code to get more information in regards to related research.

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