

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

Supplementary Material

Daniel Thürmer,¹ Orlando R. Deluigi,² Herbert M. Urbassek,³ Eduardo M. Bringa,^{2,4} and Nina Merkert¹

¹*Institute of Applied Mechanics, Clausthal University of Technology,
Adolph-Roemer Str. 2A, 38678 Clausthal-Zellerfeld, Germany*

²*CONICET and Facultad de Ingeniería, Universidad de Mendoza, Mendoza, 5500 Argentina*

³*Physics Department, University Kaiserslautern-Landau,*

Erwin-Schrödinger-Straße, D-67663 Kaiserslautern, Germany

⁴*Centro de Nanotecnología Aplicada, Facultad de Ciencias, Universidad Mayor, Santiago, Chile 8580745*

(Dated: June 7, 2024)

This Supplementary Material assembles the results for shock wave interaction with a quaternary HfNbTaZr alloy. The alloy has been modeled with the potential by Maiti and Steurer [1]. This potential has been extensively used to simulate mechanical properties, including dislocation motion [2] and tensile stress [3]. All simulation data were obtained and analyzed in analogy to the quinary HfNbTaTiZr alloy discussed in the main text.

In addition, Fig. S7 compares the pair correlation function of the hcp material in our HfNbTaTiZr sample with the one for perfect hcp. There is a reasonable match for hcp, $c/a \sim 1.63$, showing that there is no evidence for omega phase in our sample.

-
- [1] Soumyadipta Maiti and Walter Steurer, “Structural-disorder and its effect on mechanical properties in single-phase TaNbHfZr high-entropy alloy,” *Acta Materialia* **106**, 87–97 (2016).
 - [2] Shashank Mishra, Soumyadipta Maiti, and Beena Rai, “Computational property predictions of Ta–Nb–Hf–Zr high-entropy alloys,” *Scientific Reports* **11**, 4815 (2021).
 - [3] Orlando Deluigi, Felipe Valencia, Diego R. Tramontina, Nicolas Amigo, Javier Rojas-Nunez, and Eduardo M. Bringa, “Influence of grain size on mechanical properties of a refractory high entropy alloy under uniaxial tension,” *Crystals* **13**, 357 (2023).

TABLE S1. Spall strengths obtained using free surface velocity and the highest tensile stress.

U_p : piston velocity. σ_{spall} : spall strength calculated using free surface velocity. P_{zz} : minimum tensile stress measured during spall.

U_p (km/s)	σ_{spall} (GPa)	P_{zz} (GPa)
0.8	15.8	14.3
1.2	15.1	14.0
1.6	14.6	12.7

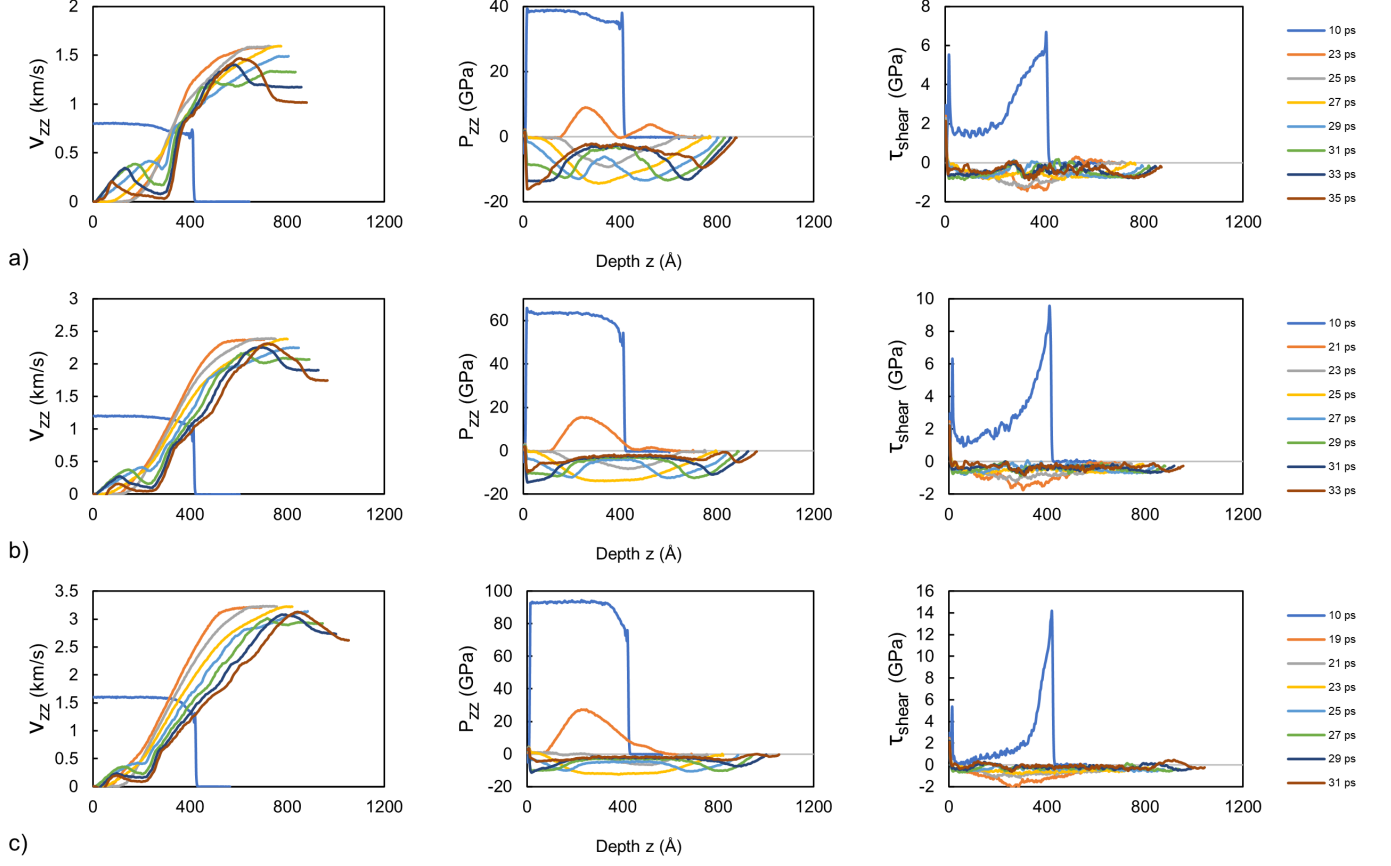


FIG. S1. Spatial profiles of the atom velocity in z direction, v_z , the normal stress parallel to the shock wave propagation direction, P_{zz} , and the shear stress, τ_{shear} , for several piston velocities: 0.8 km/s (a), 1.2 km/s (b), 1.6 km/s (c). Data are for the quaternary HfNbTaZr alloy.

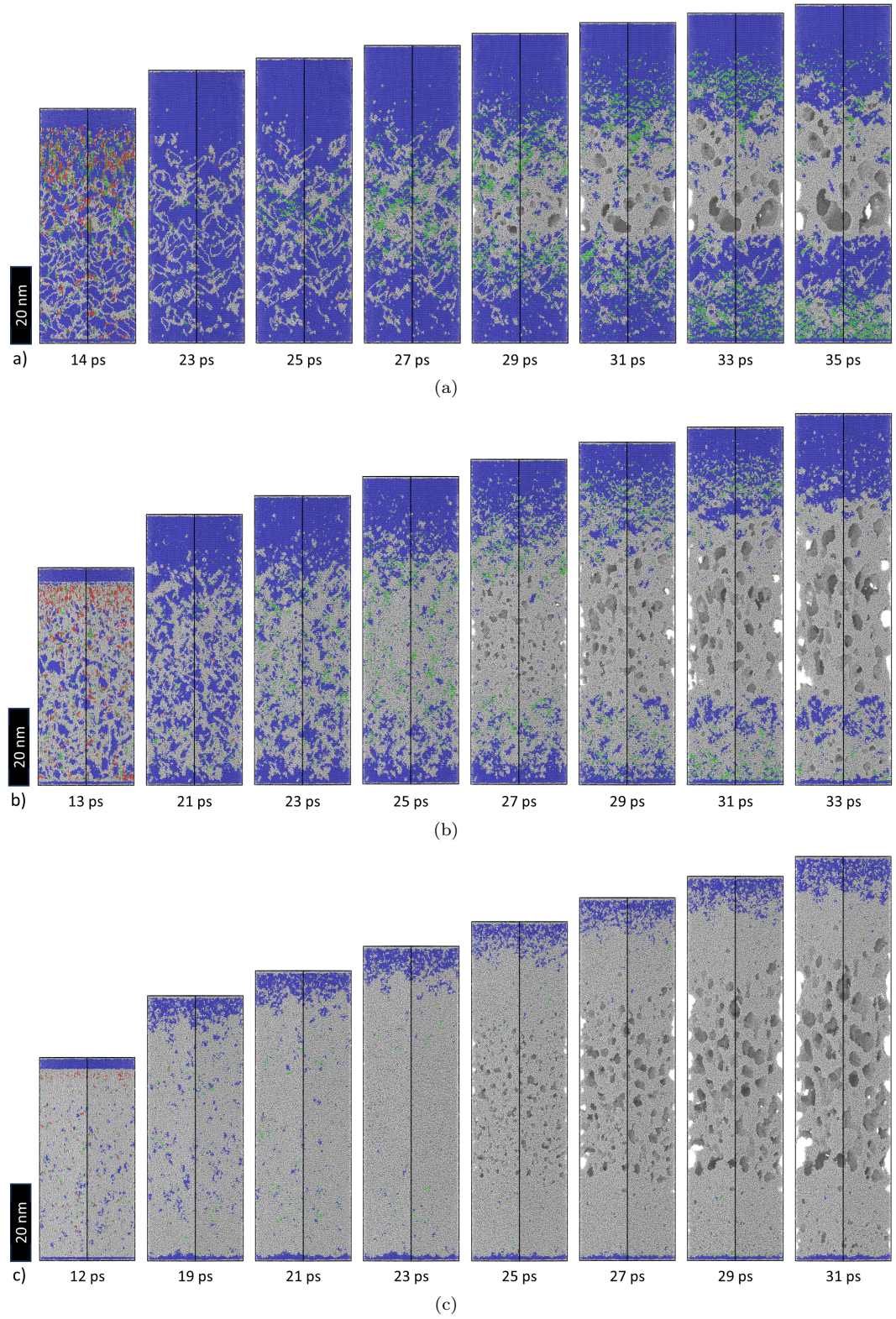


FIG. S2. Snapshots of the sample for piston velocities of (a) 0.8 km/s, (b) 1.2 km/s and (c) 1.6 km/s at various times. Atoms were identified using PTM and are colored according to their local crystal structure: green (fcc); red (hcp); blue (bcc); light gray (other). The black vertical lines denote an edge of the simulation volume. The shock propagates from bottom to top. Data are for the quaternary HfNbTaZr alloy.

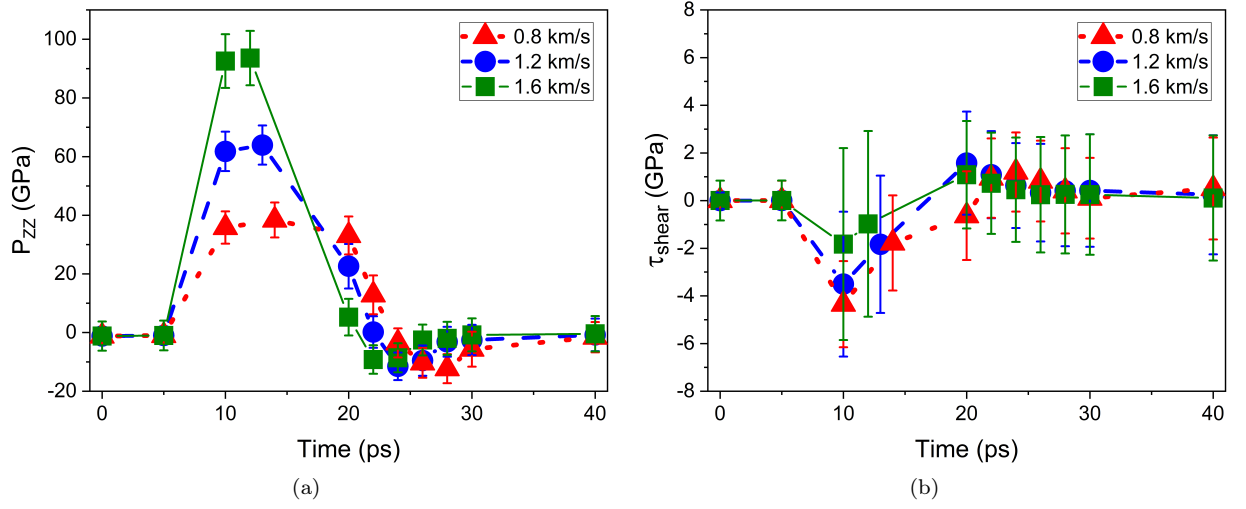


FIG. S3. Temporal evolution of the (a) normal stress parallel to the shock wave propagation direction, P_{zz} , and the (b) shear stress τ_{shear} for the various piston velocities investigated. Data are averaged over a slice of width 15 nm at the center of the sample. Data are for the quaternary HfNbTaZr alloy.

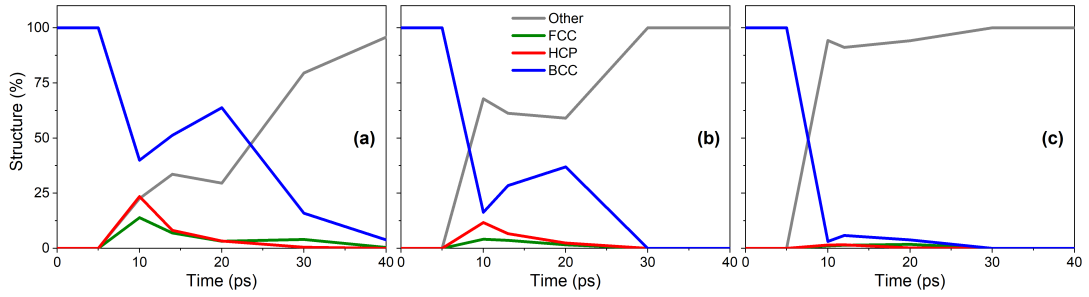


FIG. S4. Temporal evolution of the phase fraction in a slice of width 15 nm at the center of the sample. Data are for piston velocities of (a) 0.8 km/s, (b) 1.2 km/s and (c) 1.6 km/s. Atoms were identified using PTM with the parameter RMSD set to 0.1. Data are for the quaternary HfNbTaZr alloy.

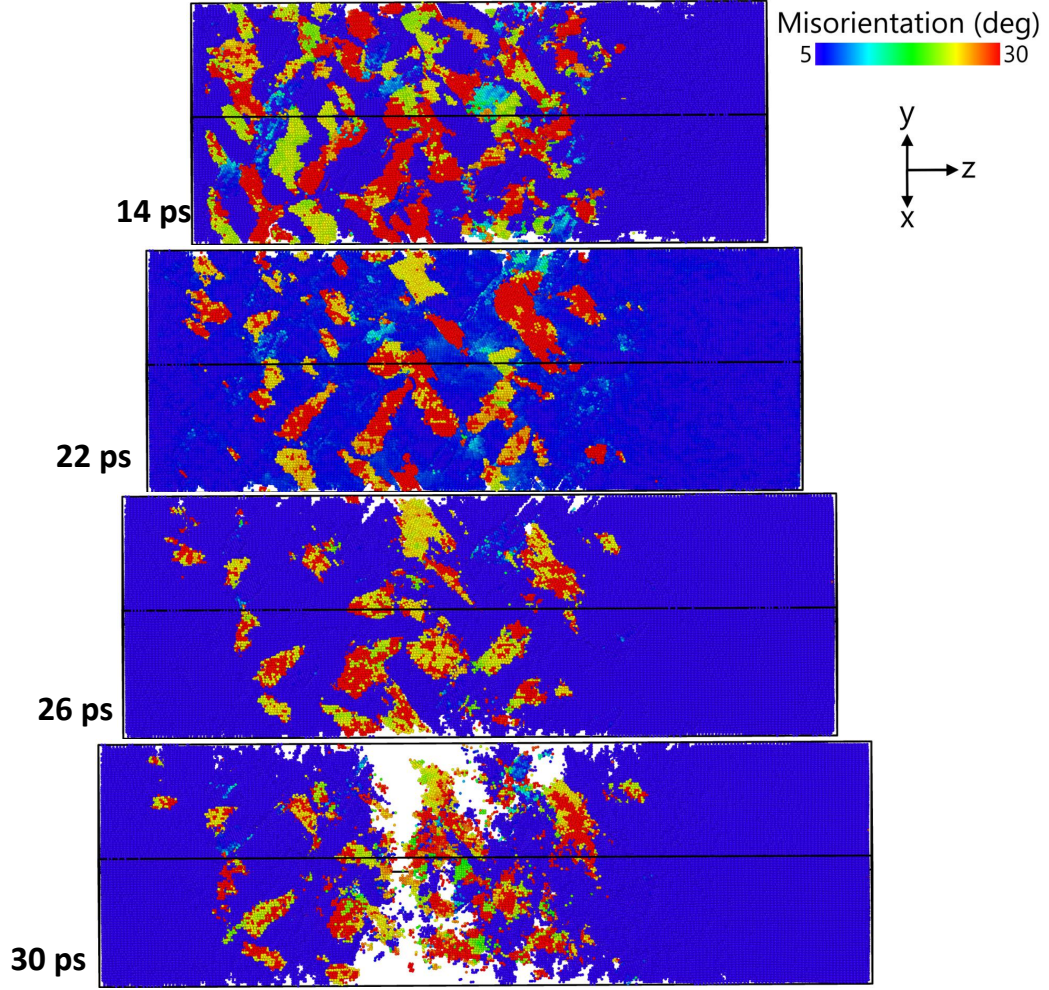


FIG. S5. Snapshots showing the twin variants developing in the bcc phase at different times for a piston velocity of 0.8 km/s. Color codes the misorientation angle to the original bcc variant. Data are for the quaternary HfNbTaZr alloy.

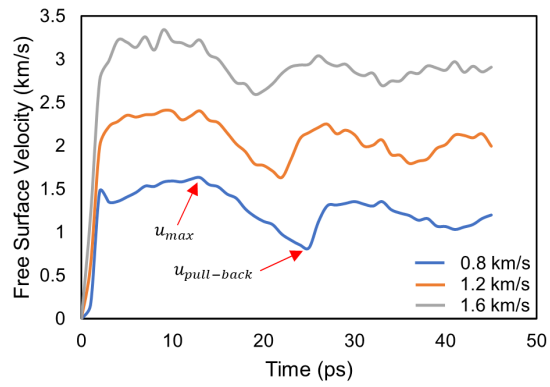


FIG. S6. Temporal evolution of the free surface velocities for the piston velocities indicated. u_{max} and $u_{pullback}$ represent the free surface velocity peak and the pull-back signal at the first minimum, respectively. Time 0 refers to the moment when the shock wave reaches the free surface.

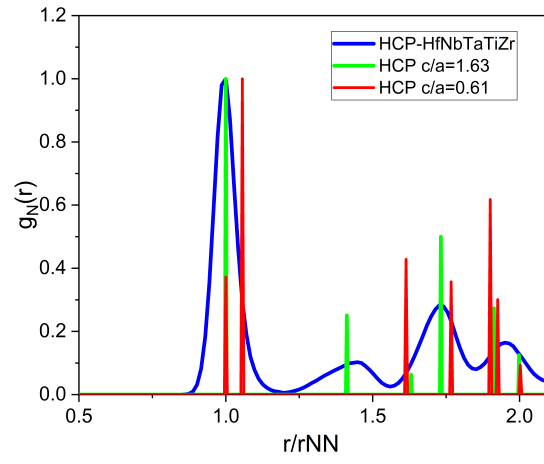


FIG. S7. Comparison between the hcp phase obtained in HfNbTaTiZr, a perfect hcp phase with $c/a = 1.63$, and a perfect omega phase with $c/a = 0.61$. The pair correlation functions $g(r)$ are plotted versus the interatomic distance r , normalized to the nearest-neighbor distance r_{NN} . Peak heights are normalized to the highest peak, which in the case of the omega phase corresponds to the second-nearest-neighbor peak.