High-velocity dust impacts in plasma facing materials: Insights from MD simulations

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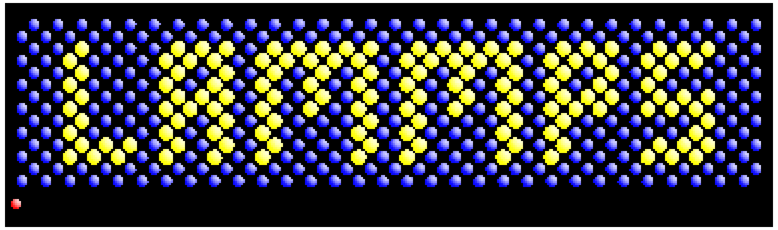

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Nuclear Fusion

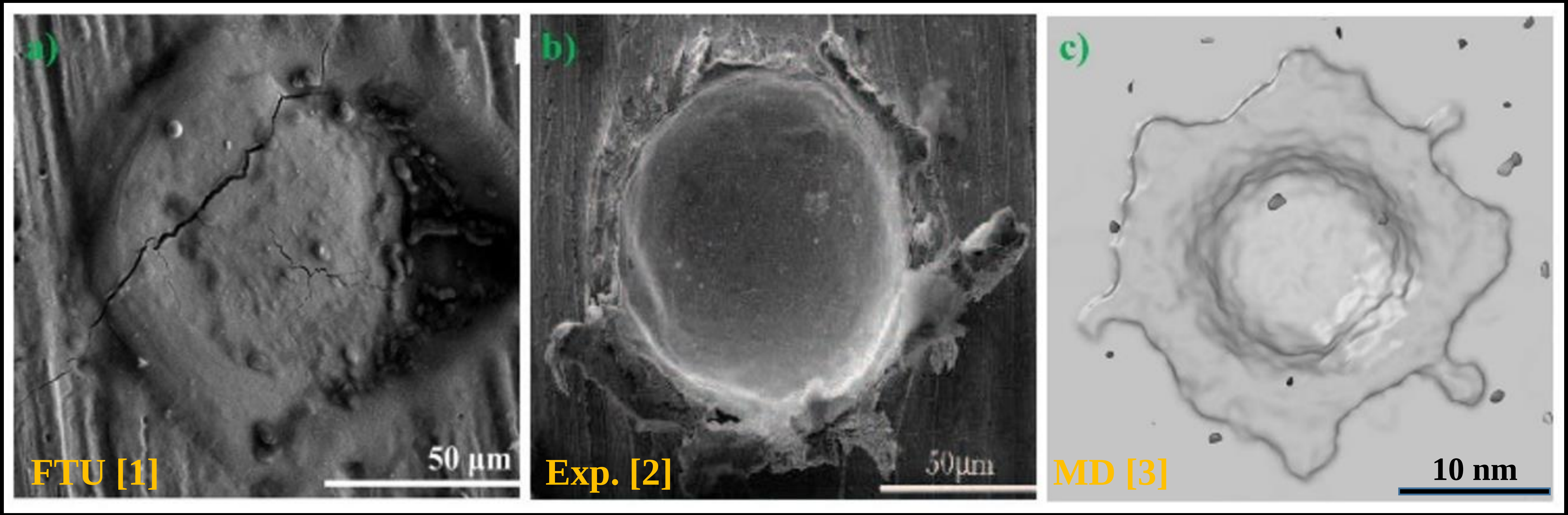
Nucl. Fusion 63 (2023) 014001 (7pp)

https://doi.org/10.1088/1741-4326/ac8a04

Letter

Evidence for high-velocity solid dust generation induced by runaway electron impact in FTU

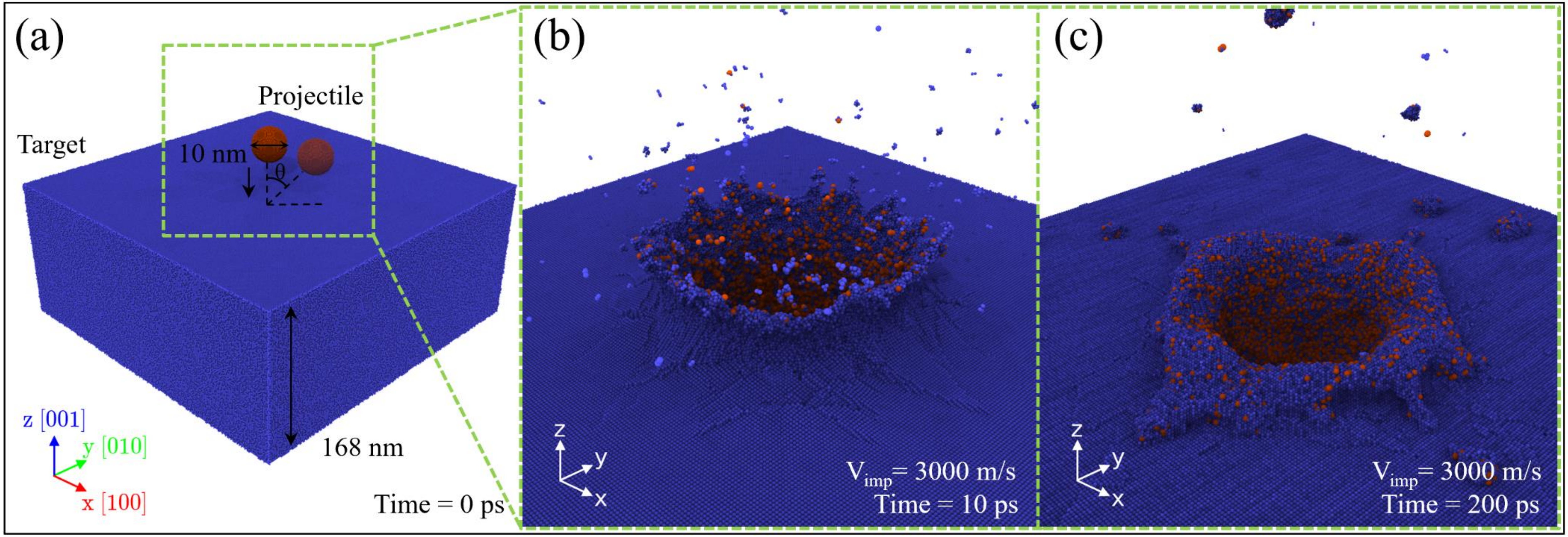
M. De Angeli[1,*], P. Tolias[2], S. Ratynskaia[2], D. Ripamonti[3], L. Vignitchouk[2], F. Causa[1], G. Daminelli[3], B. Esposito[4], E. Fortuna-Zalesna[5], F. Ghezzi[1], L. Laguardia[1], G. Maddaluno[4], G. Riva[3] and W. Zielinski[5]



[1] M. De Angeli *et al*. Nucl. Fusion 63 (2023) 014001
[2] P. Tolias *et al*. Fusion Eng. Des. 195, 113938 (2023)
[3] A. Fraile *et al*. Nucl. Fusion 62, 026034 (2022)

Can Molecular Dynamics simulate High-velocity impacts?

MD



(a)
Projectile
Target
10 nm
θ
168 nm
z [001]
y [010]
x [100]
Time = 0 ps
(b)
z
y
x
V_{imp}= 3000 m/s
Time = 10 ps
(c)
z
y
x
V_{imp}= 3000 m/s
Time = 200 ps

MD

Target: 600 x 600 x 400 A^3, (up to 200 million atoms)

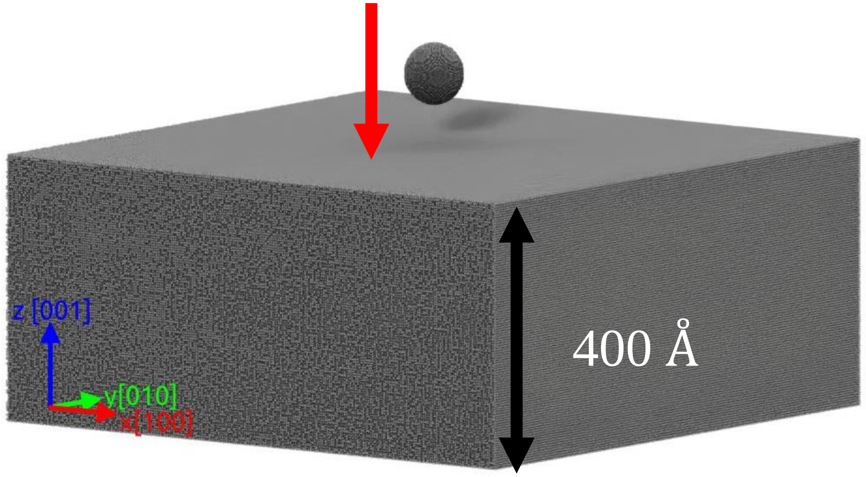
Projectiles:

- r = 4 nm 2,331, r = 8 nm, 17,261, r = 10 nm 35,000 atoms

Velocities: 1 - 4.5 km/s

Timestep: 0.1 fs

Total simulation times: 200 ps.

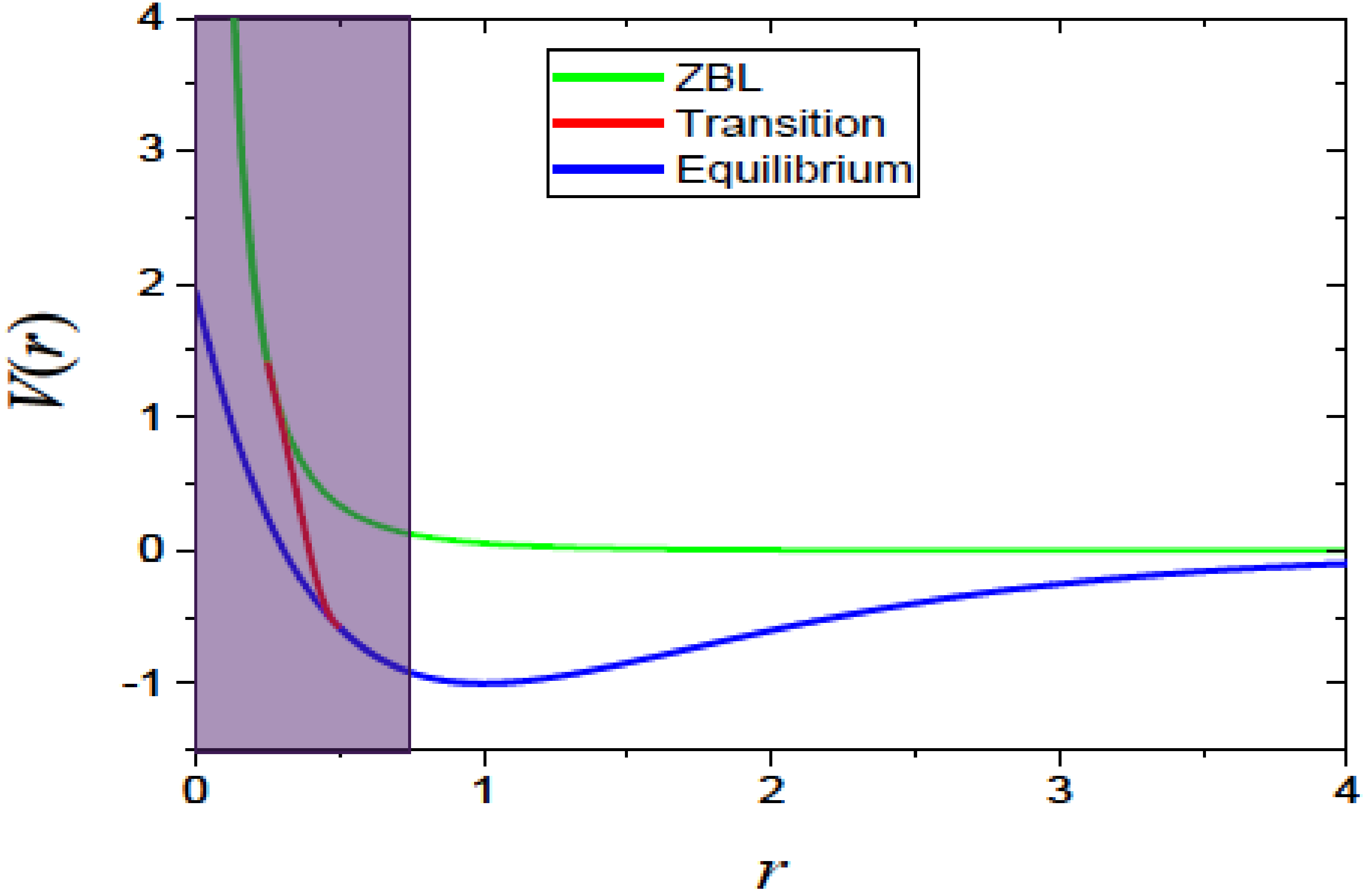


Interatomic potential: EAM, Bonny *et al.* [4].

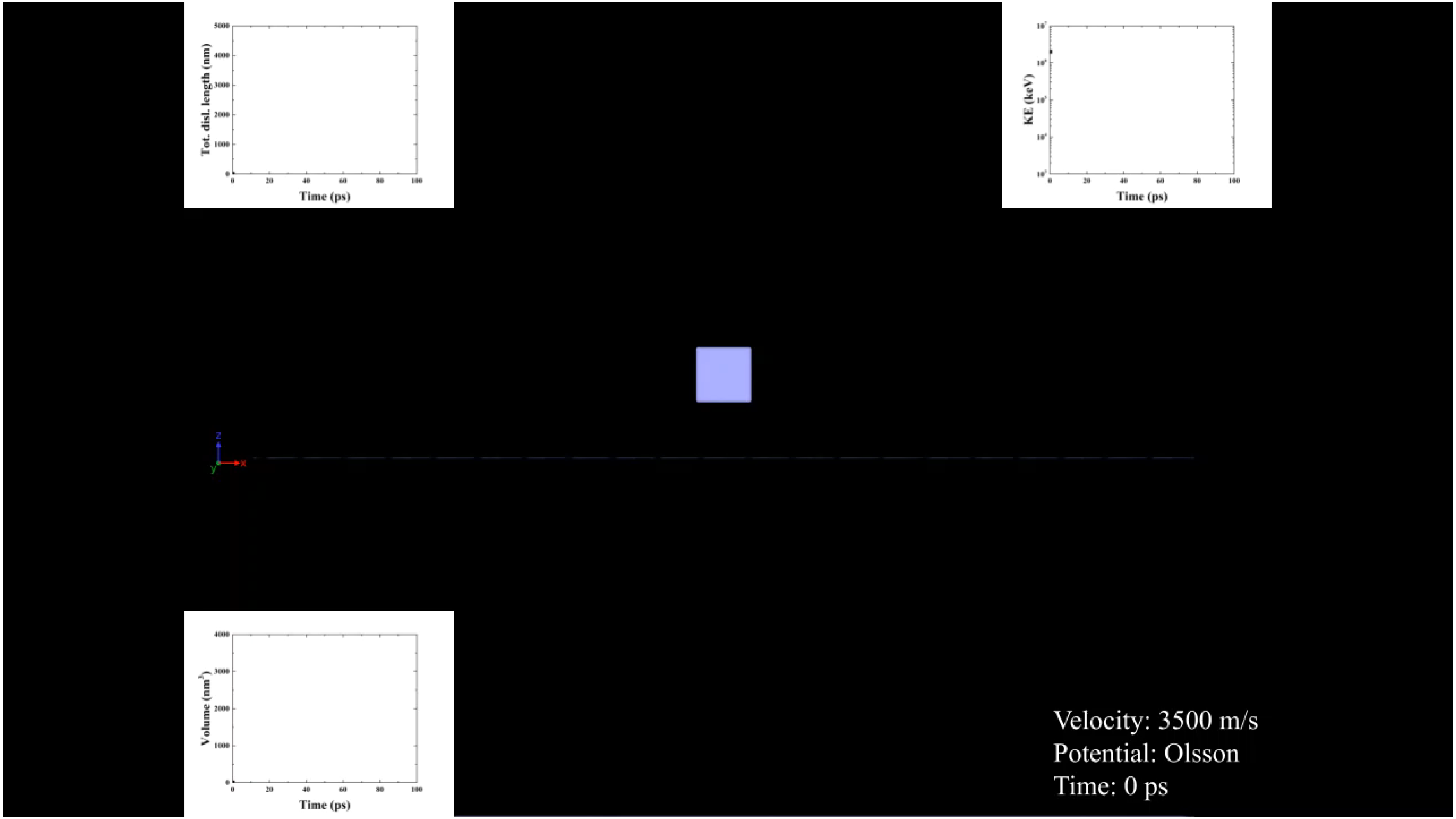
Potential joined to the universal repulsive interatomic potential of Ziegler, Biersack and Littmark [5] (**ZBL**) at small interatomic distances.

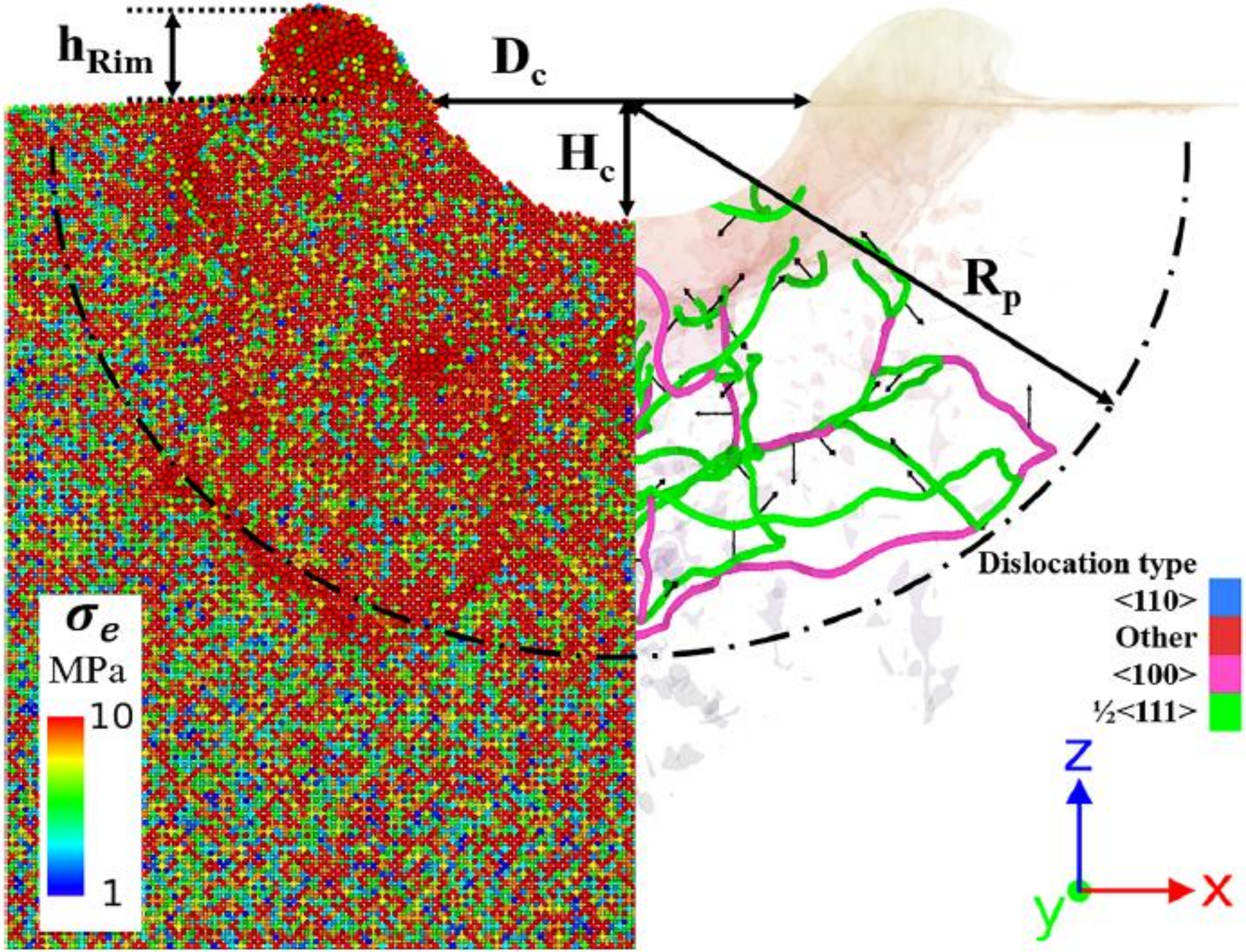
[4] G. Bonny *et al*. J. of Physics: Condensed Matter. 26, 485001 (2014).
[5] J.F. Ziegler, J.P. Biersack, and U. Littmark, The Stopping and Range of Ions in Matter, Pergamon, New York (1985).

ZBL



[5] J.F. Ziegler, J.P. Biersack, and U. Littmark, The Stopping and Range of Ions in Matter , Pergamon, New York (1985).


Tot. disl. length (nm)
0
1000
2000
3000
4000
5000
0
20
40
60
80
100
Time (ps)
KE (keV)
0
20
40
60
80
100
Time (ps)
z
x
y
Volume (nm3)
0
1000
2000
3000
4000
0
20
40
60
80
100
Time (ps)
Velocity: 3500 m/s
Potential: Olsson
Time: 0 ps



h_{Rim}
D_c
H_c
R_p
σ_e
MPa
10
1
Dislocation type
<110>
Other
<100>
½<111>
z
y
x

Π scaling theory

We used a set of scaling laws, specifically **π-group scaling laws***, to extend the findings of small-scale experiments to larger scenarios.

[*] K.A. Holsapple, The scaling of impact phenomena, Int. J. Impact Eng. 5 343–355 (1987) .
[*] K.A. Holsapple, The scaling of impact processes in planetary sciences, Annu. Rev. Earth Planet. Sci. 21, 333–373 (1993).

Π scaling theory

→ physical impact parameters → dimensionless quantities.

$$\pi_D = D_C \left(\frac{\rho_t}{m_p}\right)^{1/3}$$

[*] K.A. Holsapple, The scaling of impact phenomena, Int. J. Impact Eng. 5 343–355 (1987) .
[*] K.A. Holsapple, The scaling of impact processes in planetary sciences, Annu. Rev. Earth Planet. Sci. 21, 333–373 (1993).

Π scaling theory

→ physical impact parameters → dimensionless quantities.

$$\pi_D = D_C \left(\frac{\rho_t}{m_p}\right)^{1/3} \qquad \pi_H = H_C \left(\frac{\rho_t}{m_p}\right)^{1/3}$$

[*] K.A. Holsapple, The scaling of impact phenomena, Int. J. Impact Eng. 5 343–355 (1987) .
[*] K.A. Holsapple, The scaling of impact processes in planetary sciences, Annu. Rev. Earth Planet. Sci. 21, 333–373 (1993).

Π scaling theory

→ physical impact parameters → dimensionless quantities.

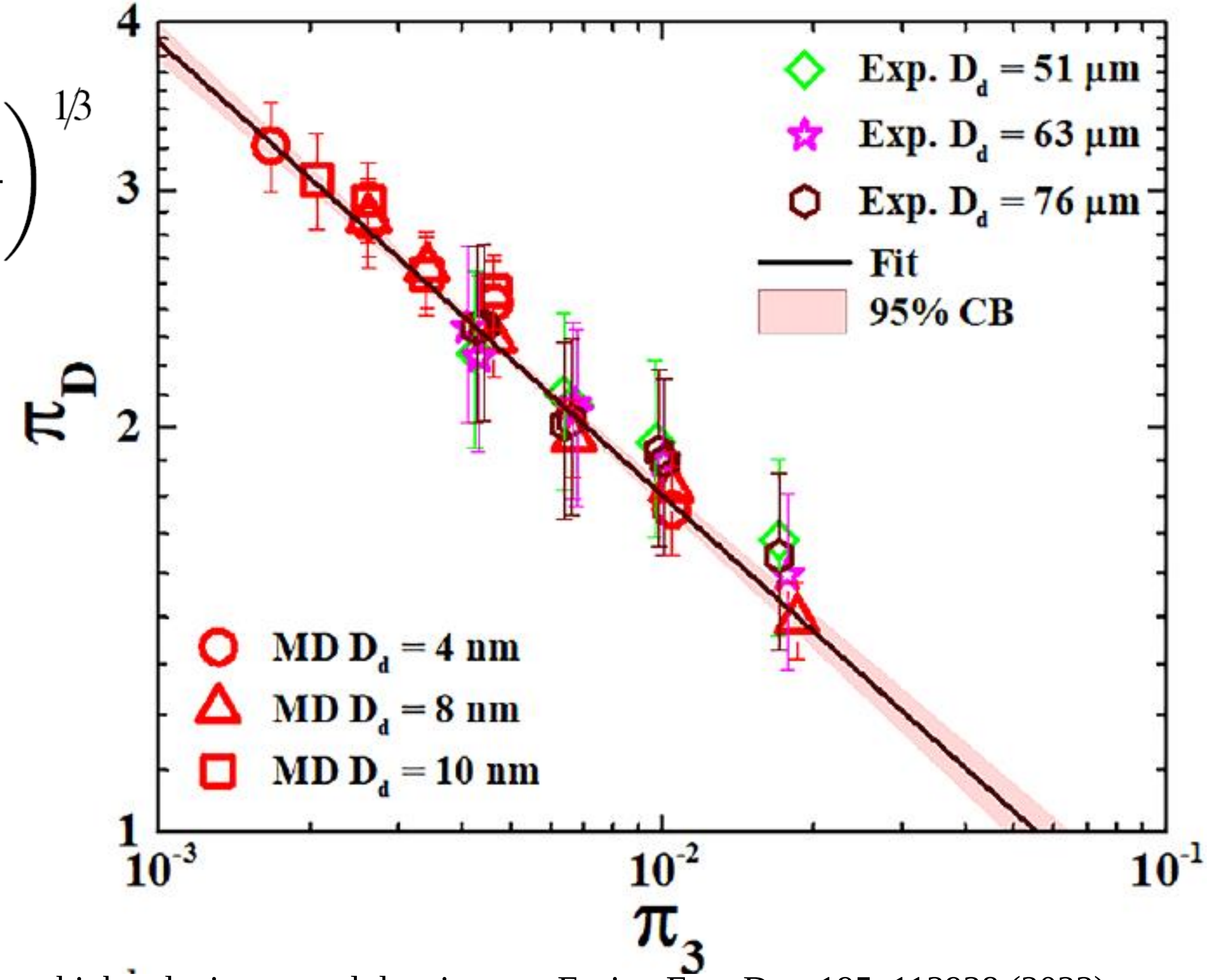
$$\pi_D = D_C \left(\frac{\rho_t}{m_p}\right)^{1/3} \qquad \pi_H = H_C \left(\frac{\rho_t}{m_p}\right)^{1/3} \qquad \pi_V = \frac{\rho_t V_C}{m_p}$$

[*] K.A. Holsapple, The scaling of impact phenomena, Int. J. Impact Eng. 5 343–355 (1987) .

[*] K.A. Holsapple, The scaling of impact processes in planetary sciences, Annu. Rev. Earth Planet. Sci. 21, 333–373 (1993).

$$\pi_D = D_C \left(\frac{\rho_t}{m_p}\right)^{1/3}$$

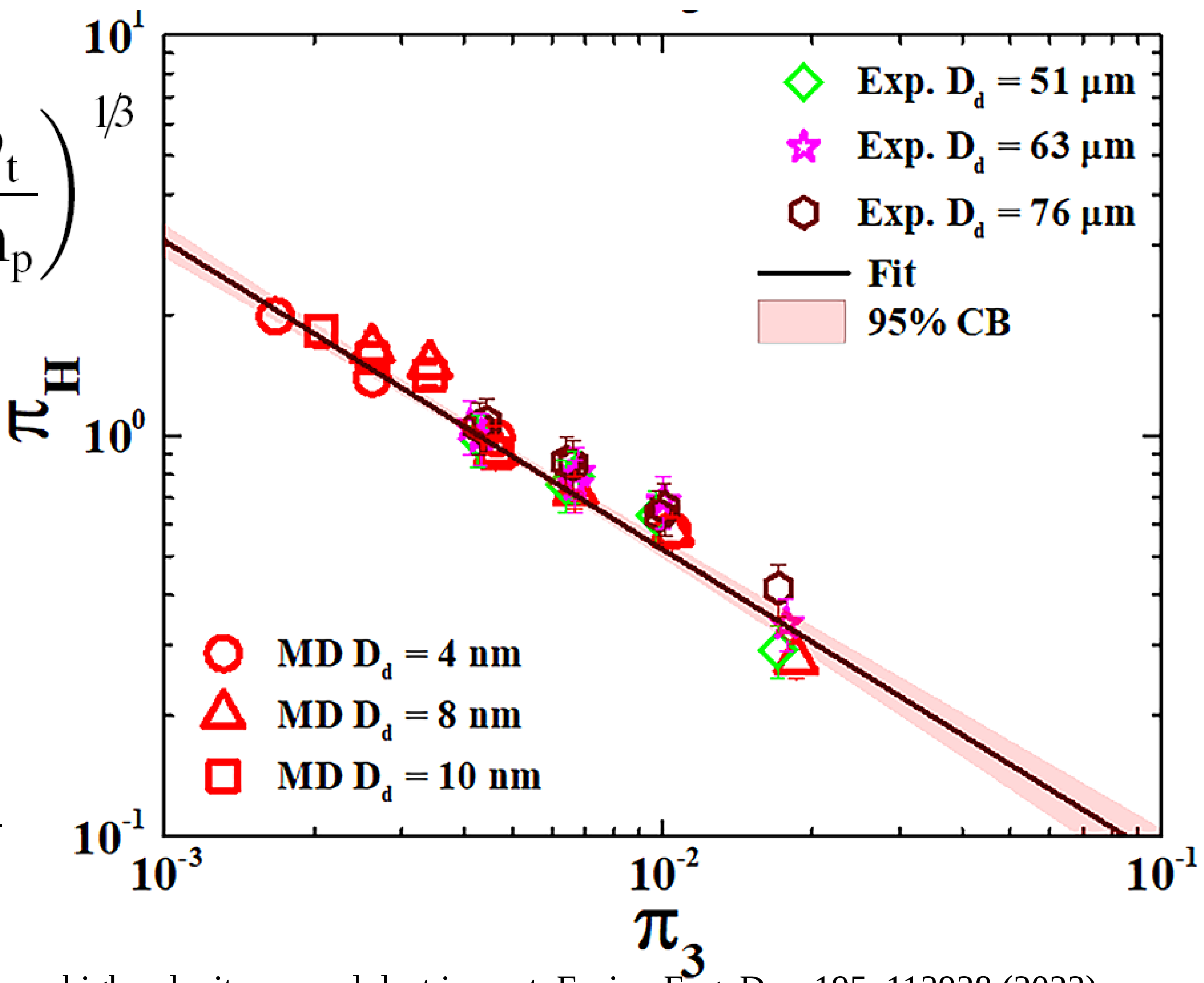
$$\pi_3 = \frac{Y_s}{\rho_p V_{imp}^2}$$



P. Tolias *et al*. Wall cratering upon high velocity normal dust impact, Fusion Eng. Des. 195, 113938 (2023)

$$\pi_H = H_C \left(\frac{\rho_t}{m_p} \right)^{1/3}$$

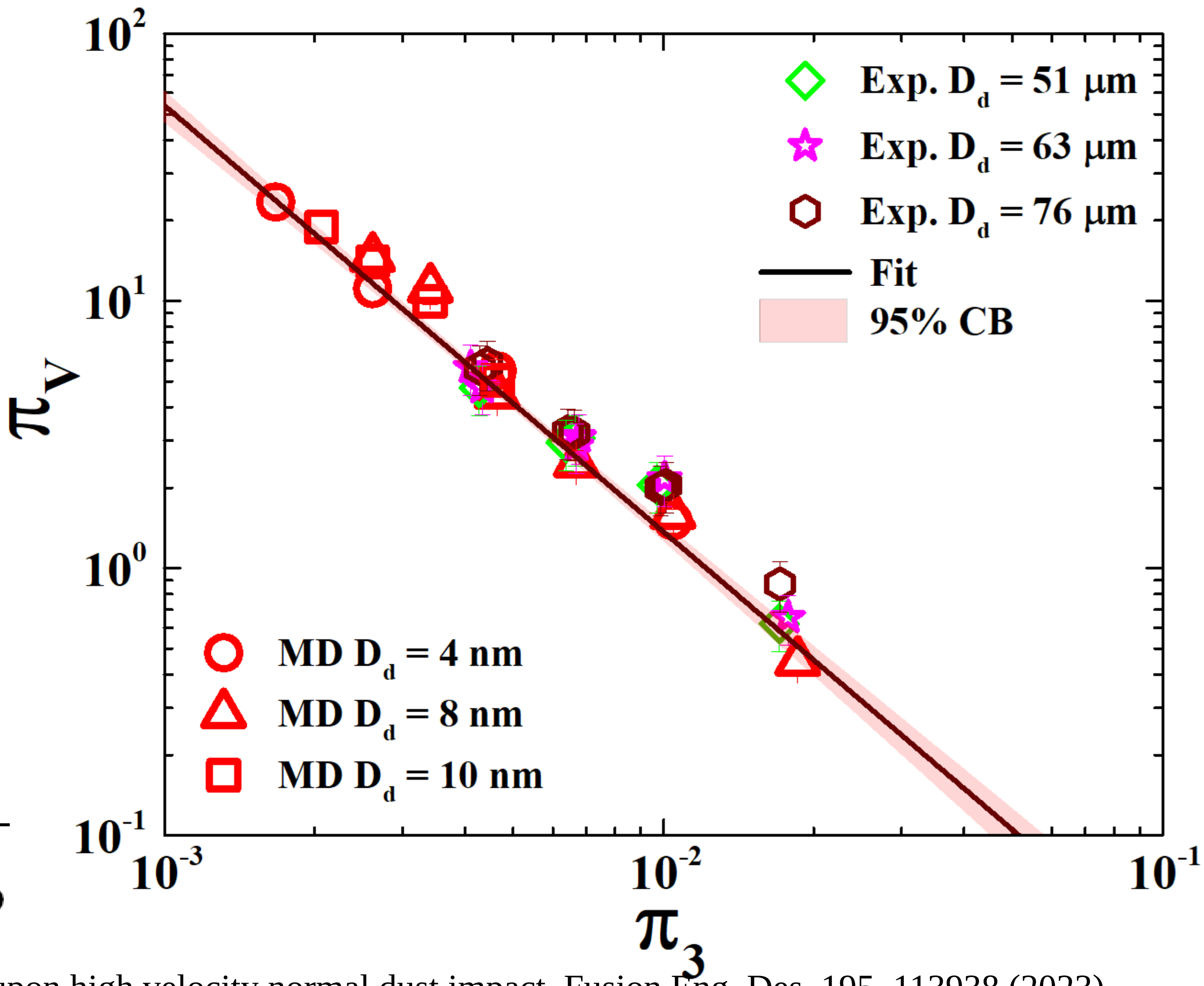
$$\pi_3 = \frac{Y_s}{\rho_p V_{imp}^2}$$



P. Tolias *et al*. Wall cratering upon high velocity normal dust impact, Fusion Eng. Des. 195, 113938 (2023)

$$\pi_V = \frac{\rho_t V_C}{m_p}$$

$$\pi_3 = \frac{Y_s}{\rho_p V_{imp}^2}$$



P. Tolias *et al*. Wall cratering upon high velocity normal dust impact, Fusion Eng. Des. 195, 113938 (2023)

In the strength regime [1, 2] (gravity is negligible)

$$\pi_H = k_H \pi_3^{-\gamma_H}$$

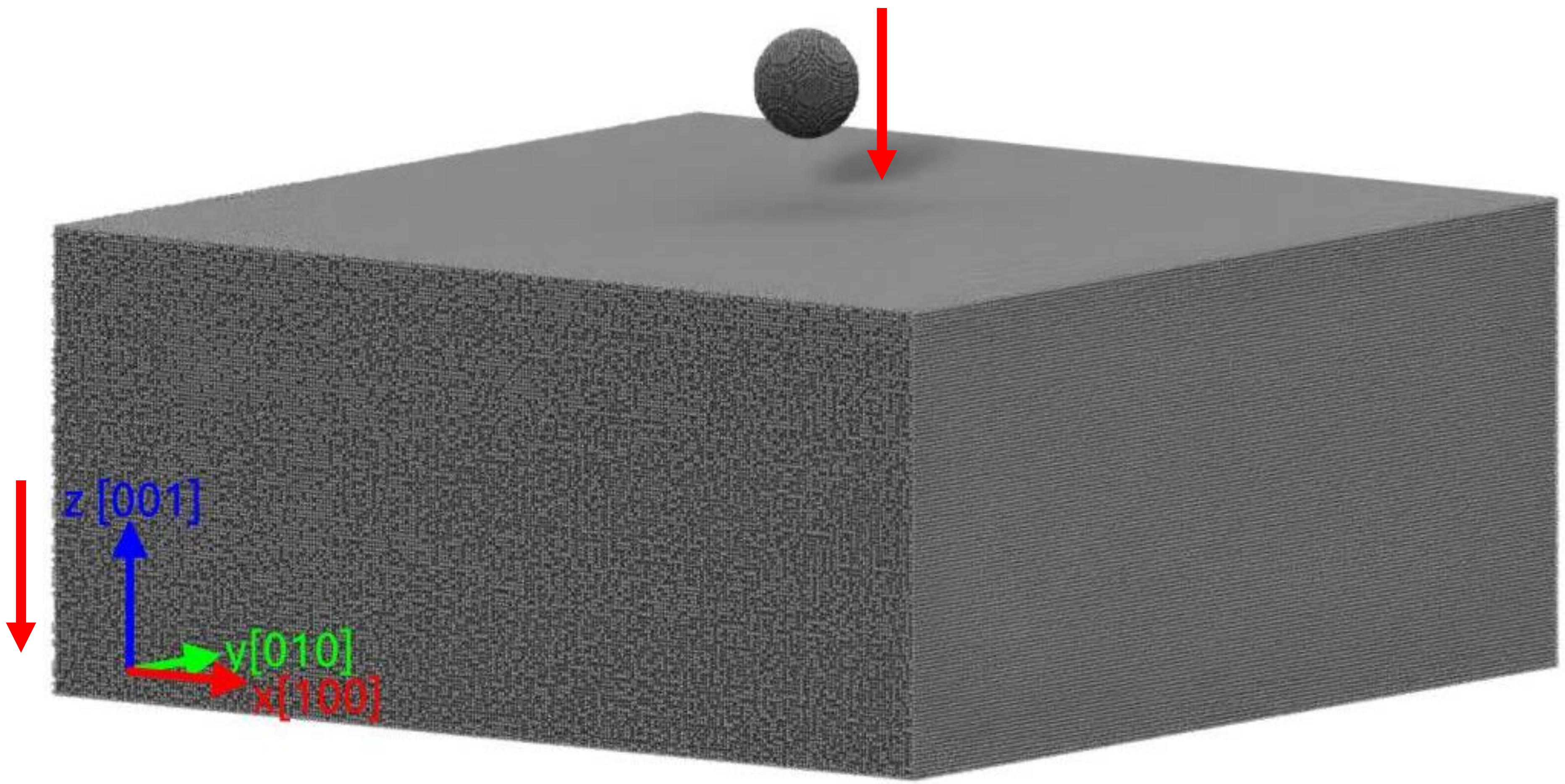
$$\pi_D = k_D \pi_3^{-\gamma_D}$$

$$\pi_V = k_V \pi_3^{-\gamma_V}$$

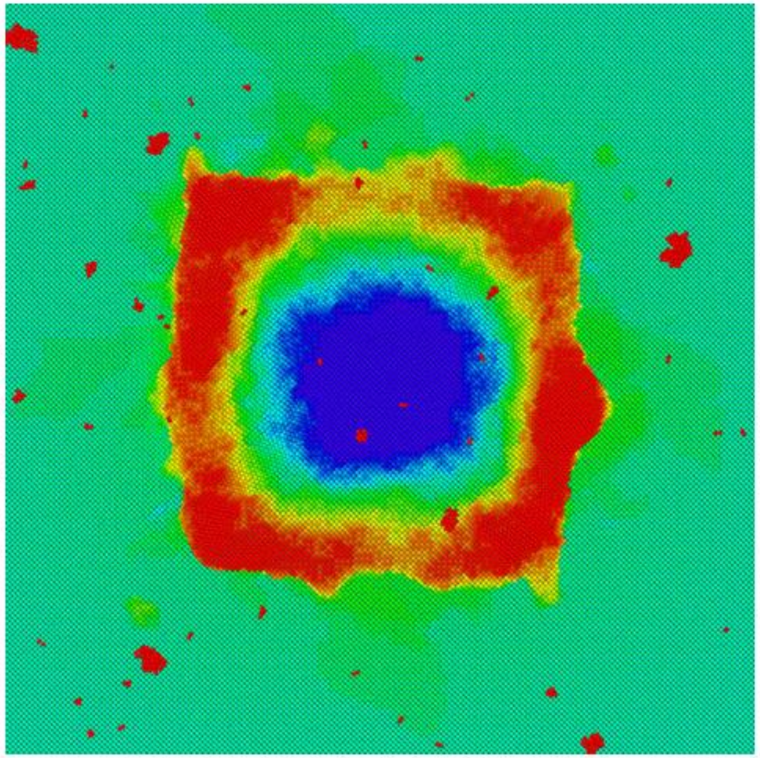
Projectile	Target	k_D	γ_D	k_H	γ_H	k_V	γ_V	Ref
W	**W**	0.37	-0.33	0.01	-0.76	0.0008	-1.5	This work
SS	**SS**	0.062	-0.26	0.78	-0.45	0.003	-0.97	[3]

[1] K. A. Holsapple. J. Geophys. Res. Solid Earth. 92 6350 (1987)
[2] R. M. Schmidt. Int. J. Impact Eng. 5, 543–560 (1987).
[3] R. Ogawa, *et al*. Icarus 362 (2021) 114410

Xtal Orientation



Xtal Orientation



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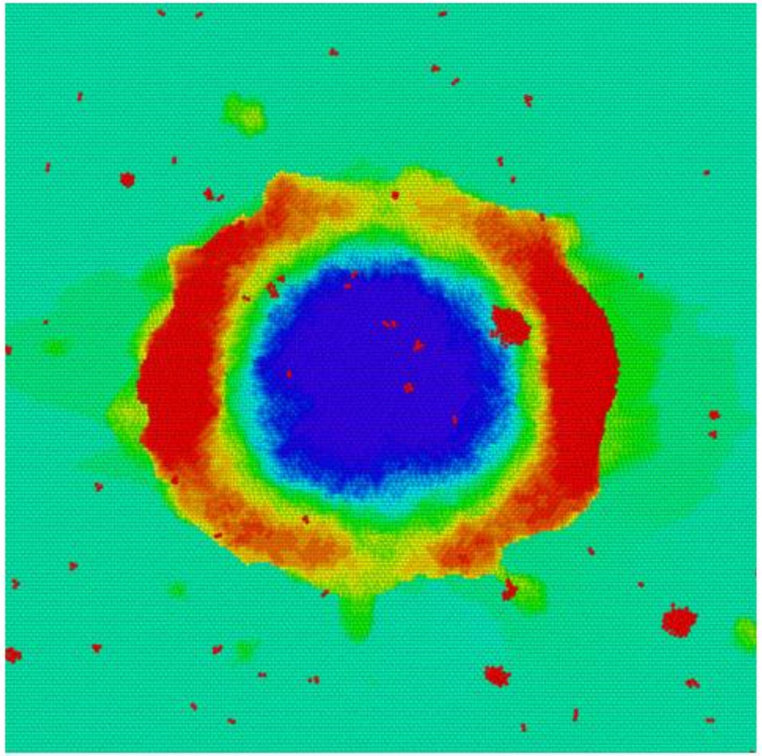
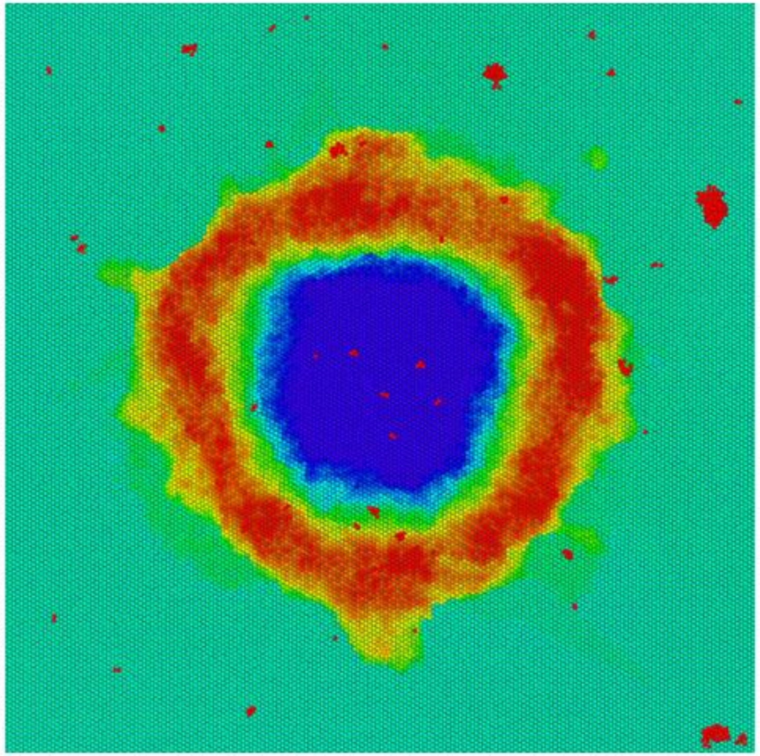
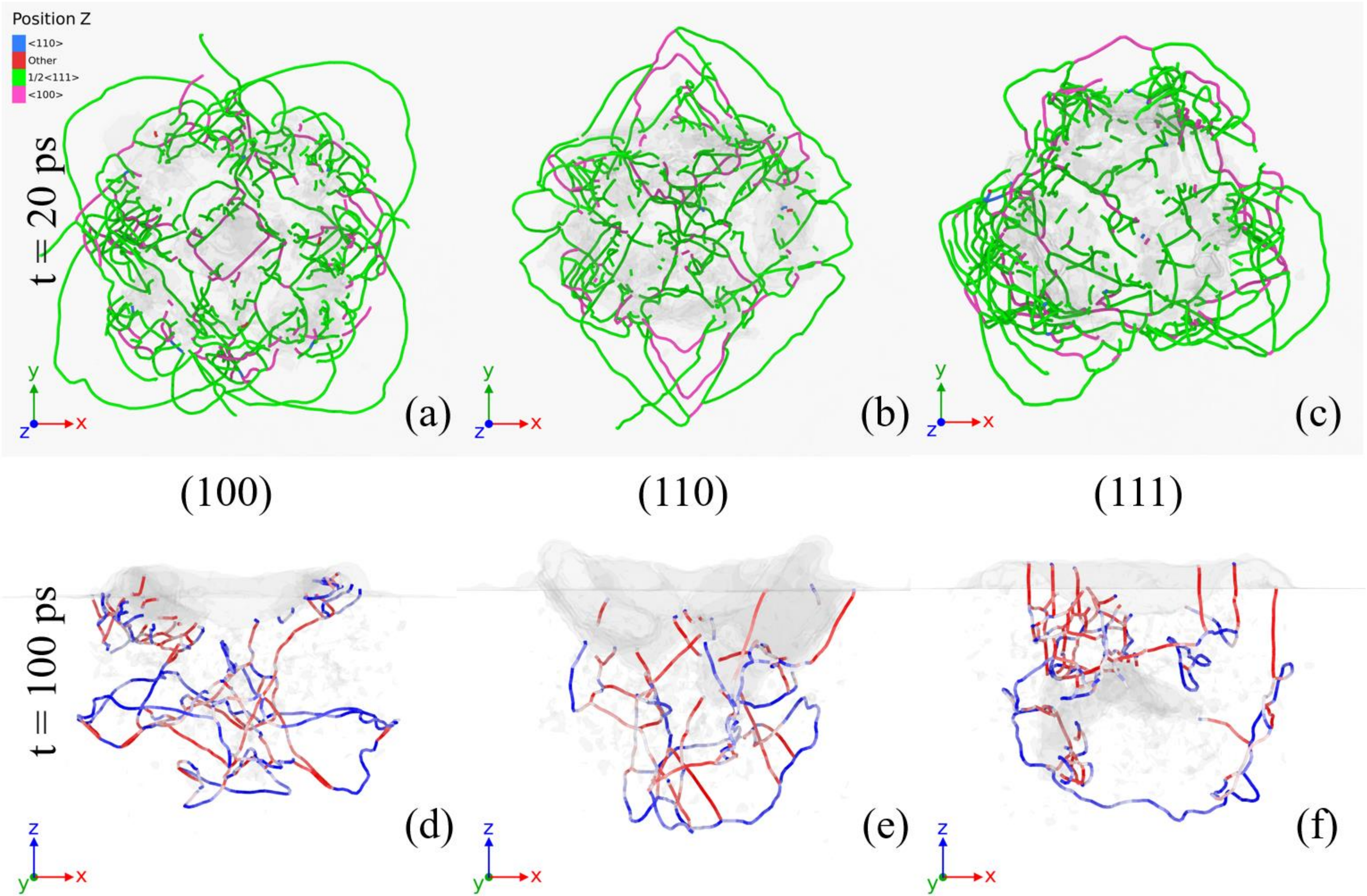


110

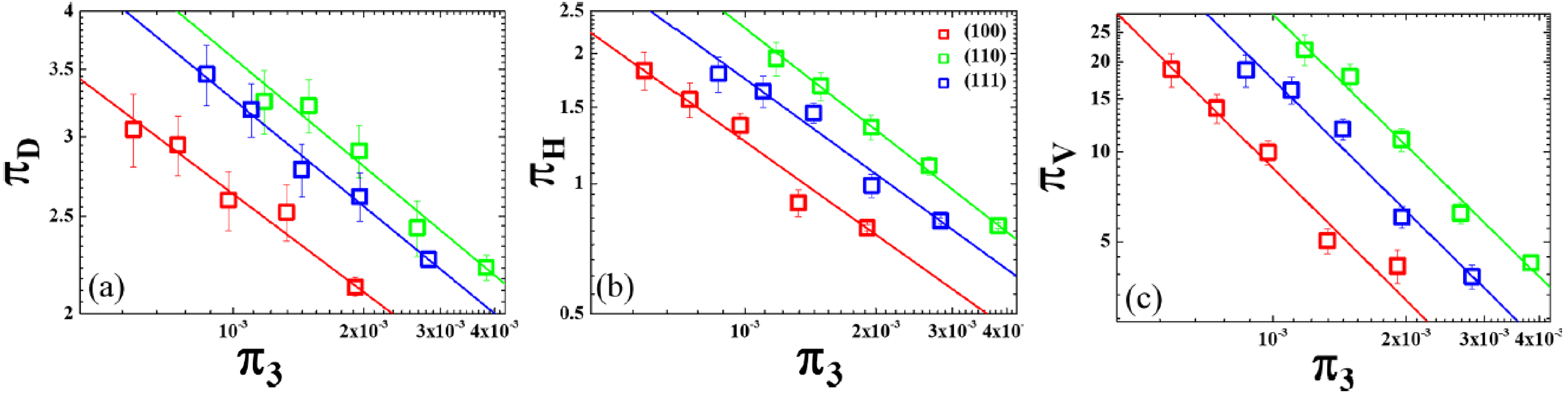


111



Position Z
<110>
Other
1/2<111>
<100>
t = 20 ps
t = 100 ps
(a)
(b)
(c)
(d)
(e)
(f)
(100)
(110)
(111)
y
x
z

Xtal Orientation

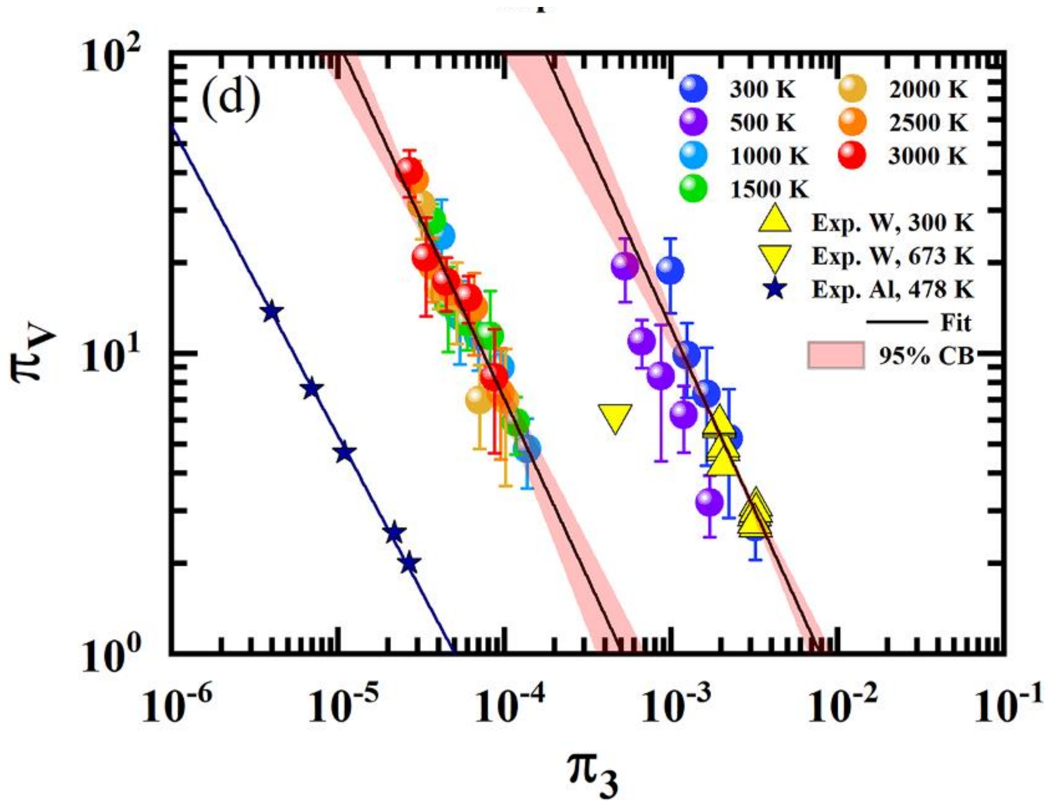


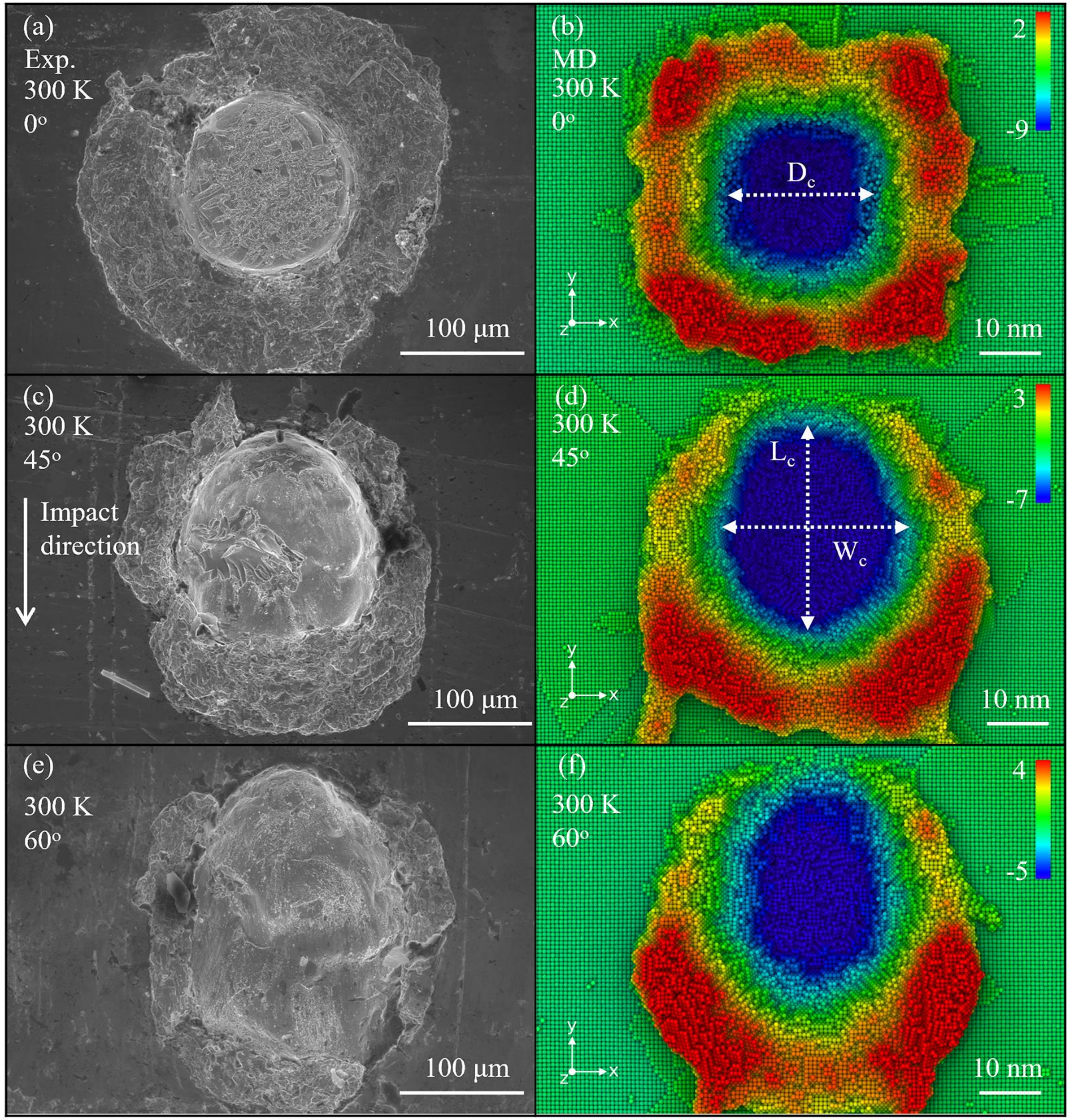
	100	110	111	Ref
Y_S (MPa)	230	460	339	[1]

	(100)	(110)	(111)
Y_s	230	460	339
k_D	0.27	0.28	0.29
k_H	0.008	0.01	0.01
k_V	0.00034	0.00072	0.0012
$k_{Hc/Dc}$	0.03	0.03	0.03
γ_D	−0.32	−0.32	−0.35
γ_H	−0.71	−0.72	−0.78
γ_V	−1.46	−1.46	−1.45
$\gamma_{Hc/Dc}$	−0.38	−0.39	−0.42

[1] A.S. Argon *et al*. Acta Metall. 14, 1449–1462 (1966)

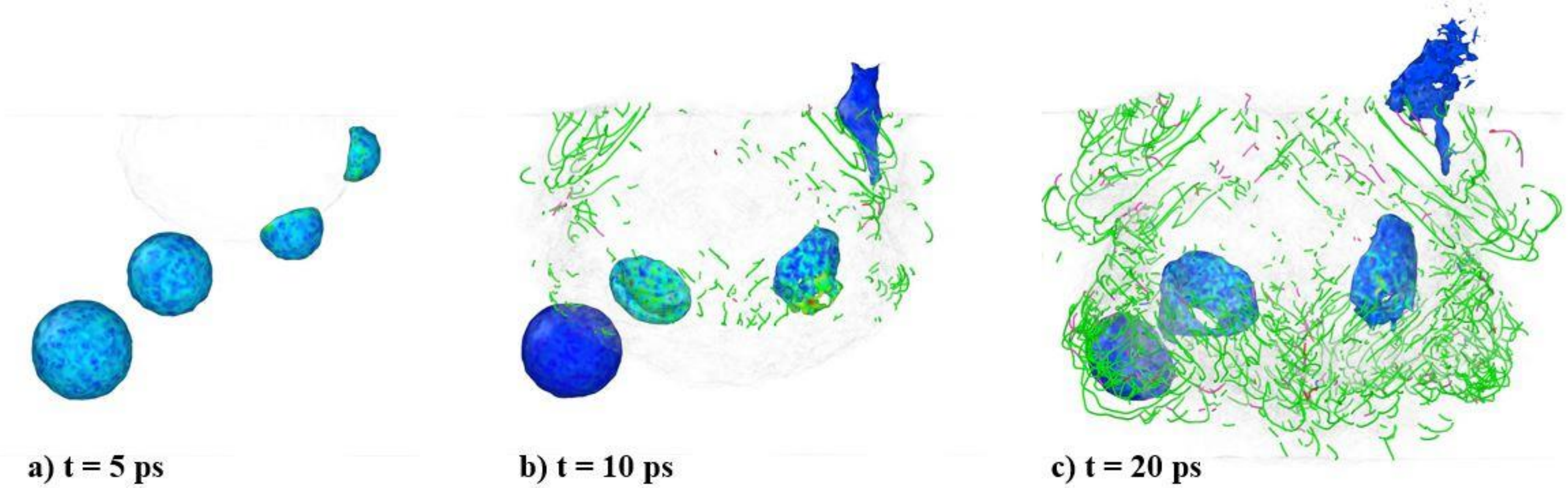
Temp. & Angle



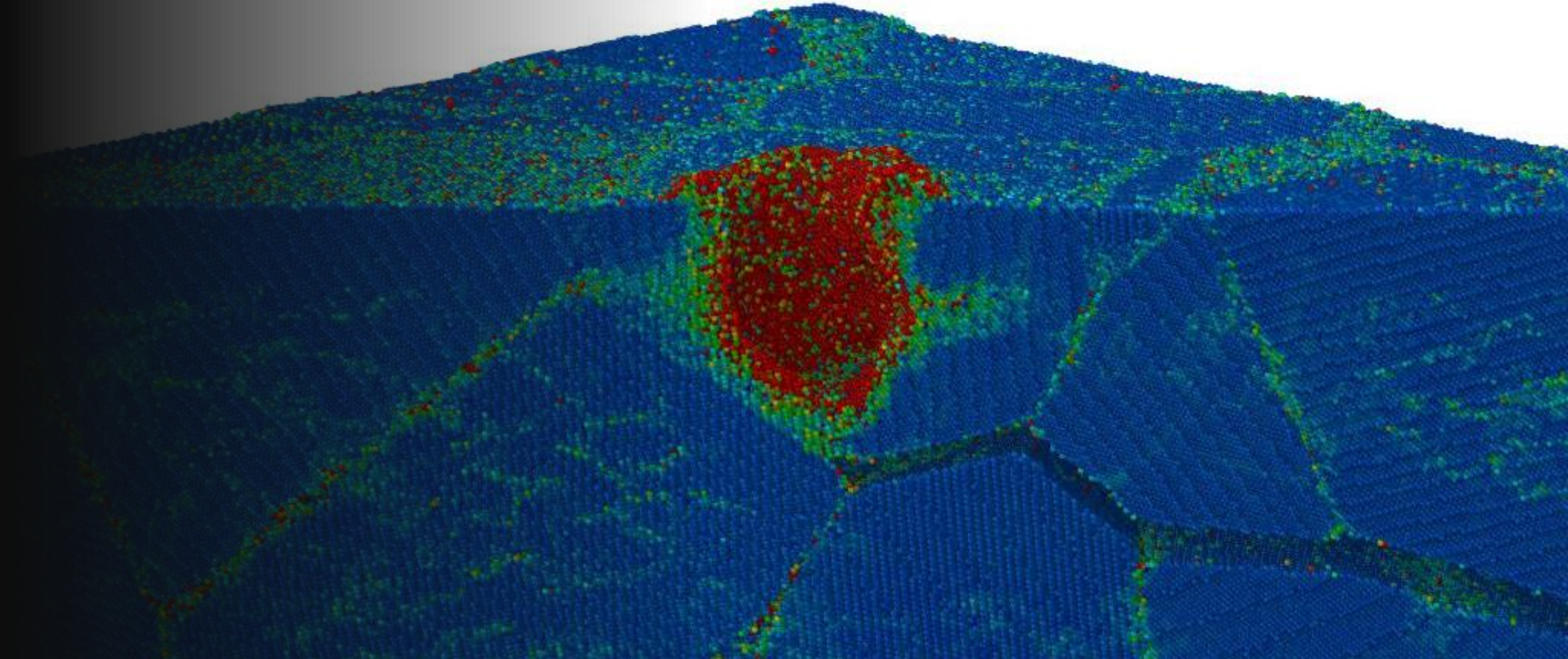


[2] P. Dwivedi, A. Fraile, T. Polcar. J. Nucl. Mater. 600, 155289 (2024)

In progress: He bubbles



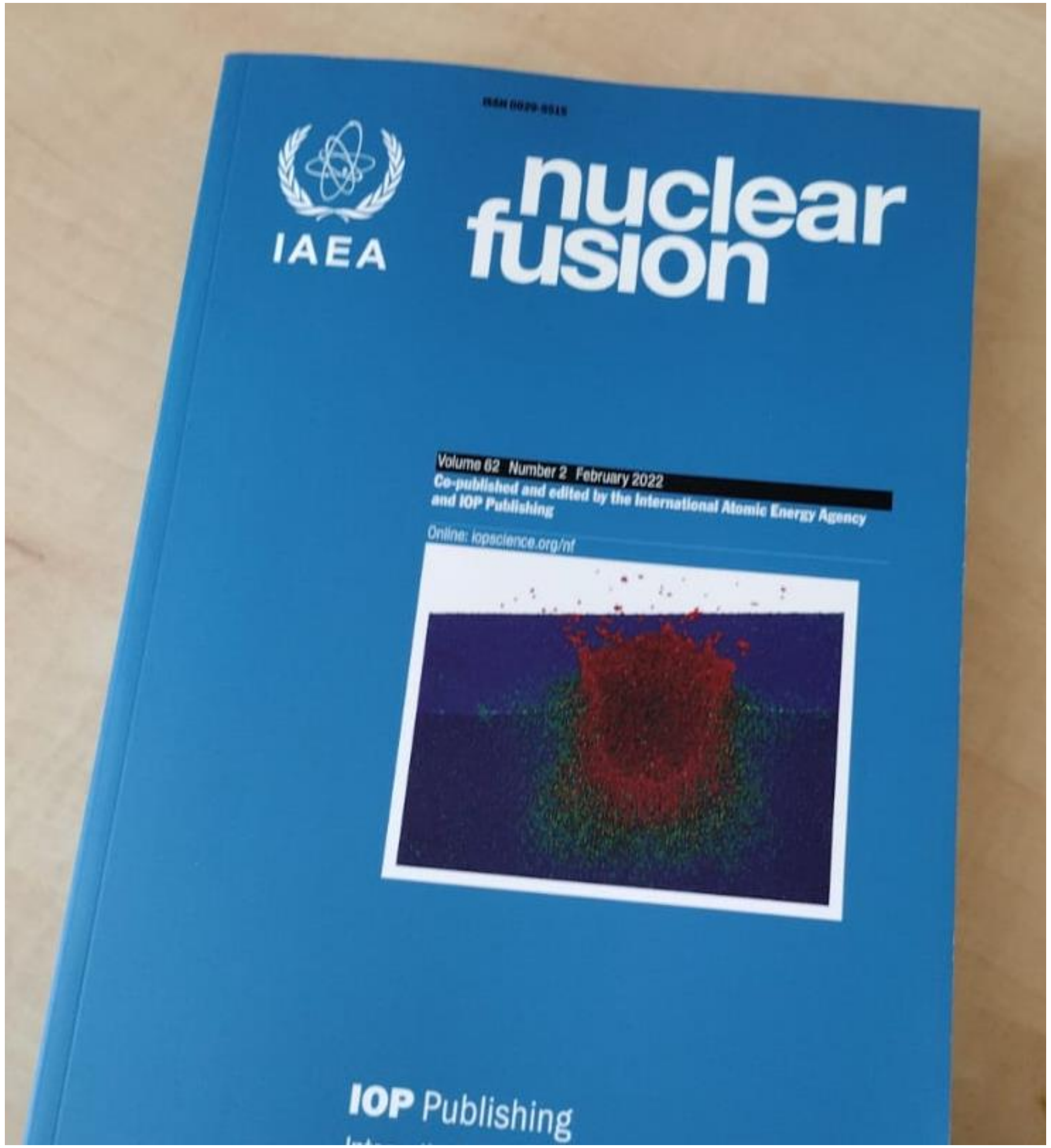
In progress



[1] A. Fraile, P. Dwivedi, G. Bonny, T. Polcar, Nuclear Fusion. 62, 026034 (2022)

[2] P. Dwivedi, A. Fraile, T. Polcar. J. Nucl. Mater. 594, 155042 (2024)

[3] P. Dwivedi, A. Fraile, T. Polcar. J. Nucl. Mater. 600, 155289 (2024)



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Thank you for your attention

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de Nanociència
i Nanotecnologia

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UNIVERSITY
IN PRAGUE

Thanks to:

Prashant Dwivedi, Tomas Polcar
Marco De Angeli

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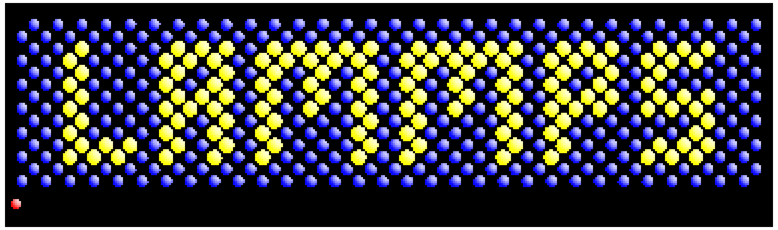

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Journal of Nuclear Materials 594 (2024) 155042

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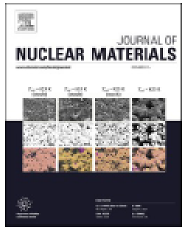

High-velocity dust impacts in plasma facing materials: Insights from molecular dynamics simulations

Prashant Dwivedi [a,*], Alberto Fraile [b,c], Tomas Polcar [a]

Journal of Nuclear Materials 600 (2024) 155289

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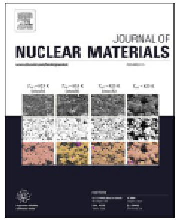
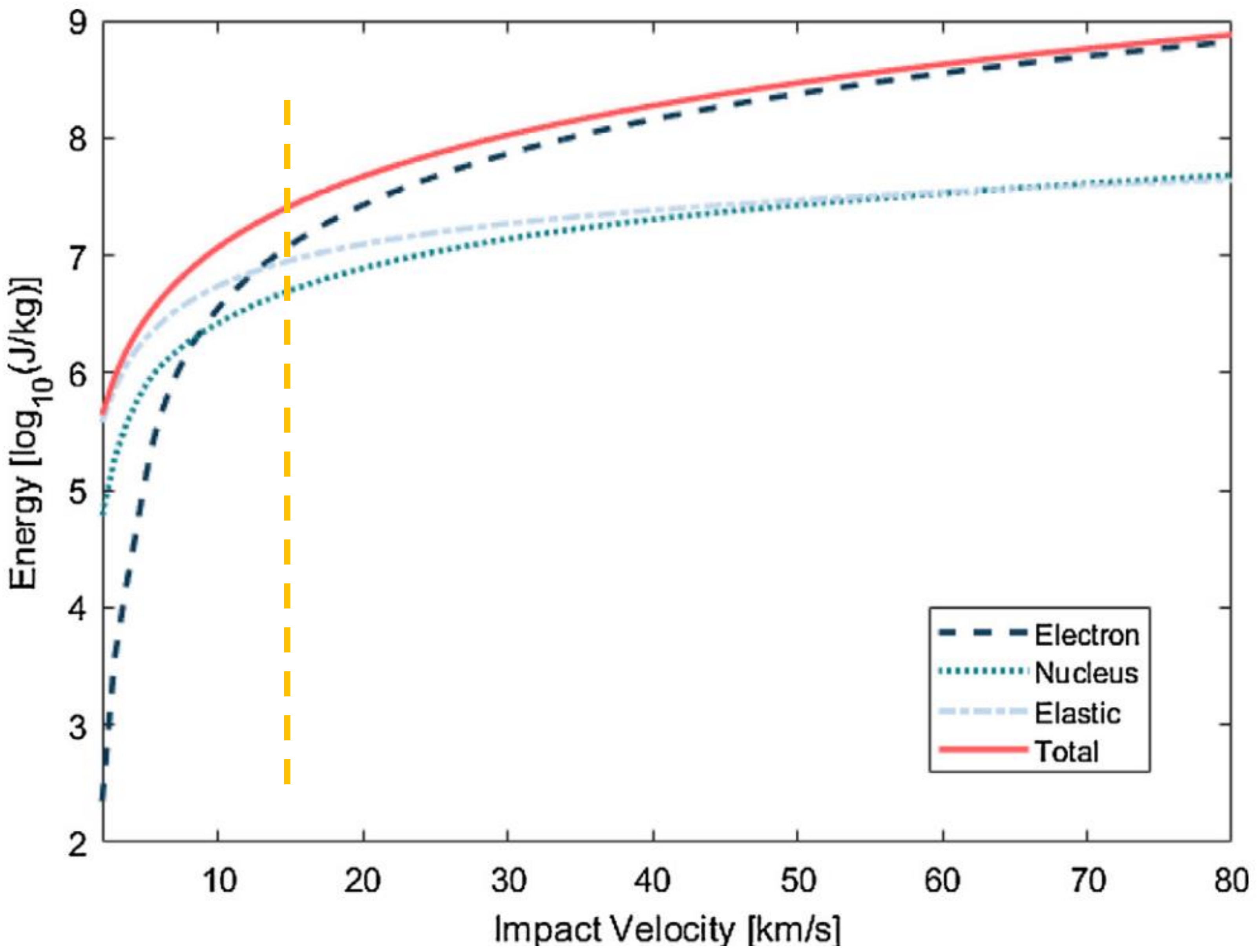


Tungsten wall cratering under high-velocity dust impacts: Influence of impact angle and temperature

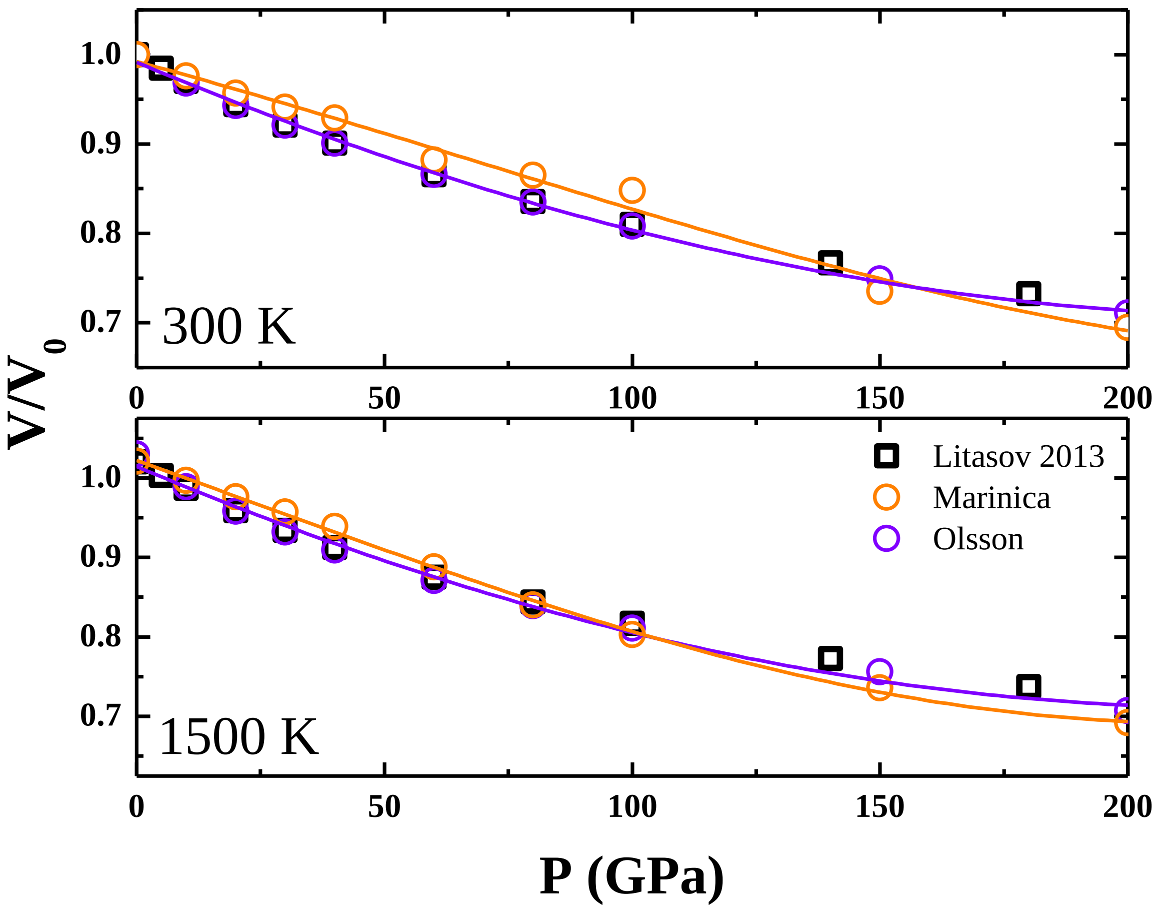
P. Dwivedi [a,*], A. Fraile [b], T. Polcar [a]

[2] P. Dwivedi, A. Fraile, T. Polcar. J. Nucl. Mater. 594, 155042 (2024)
[3] P. Dwivedi, A. Fraile, T. Polcar. J. Nucl. Mater. 600, 155289 (2024)

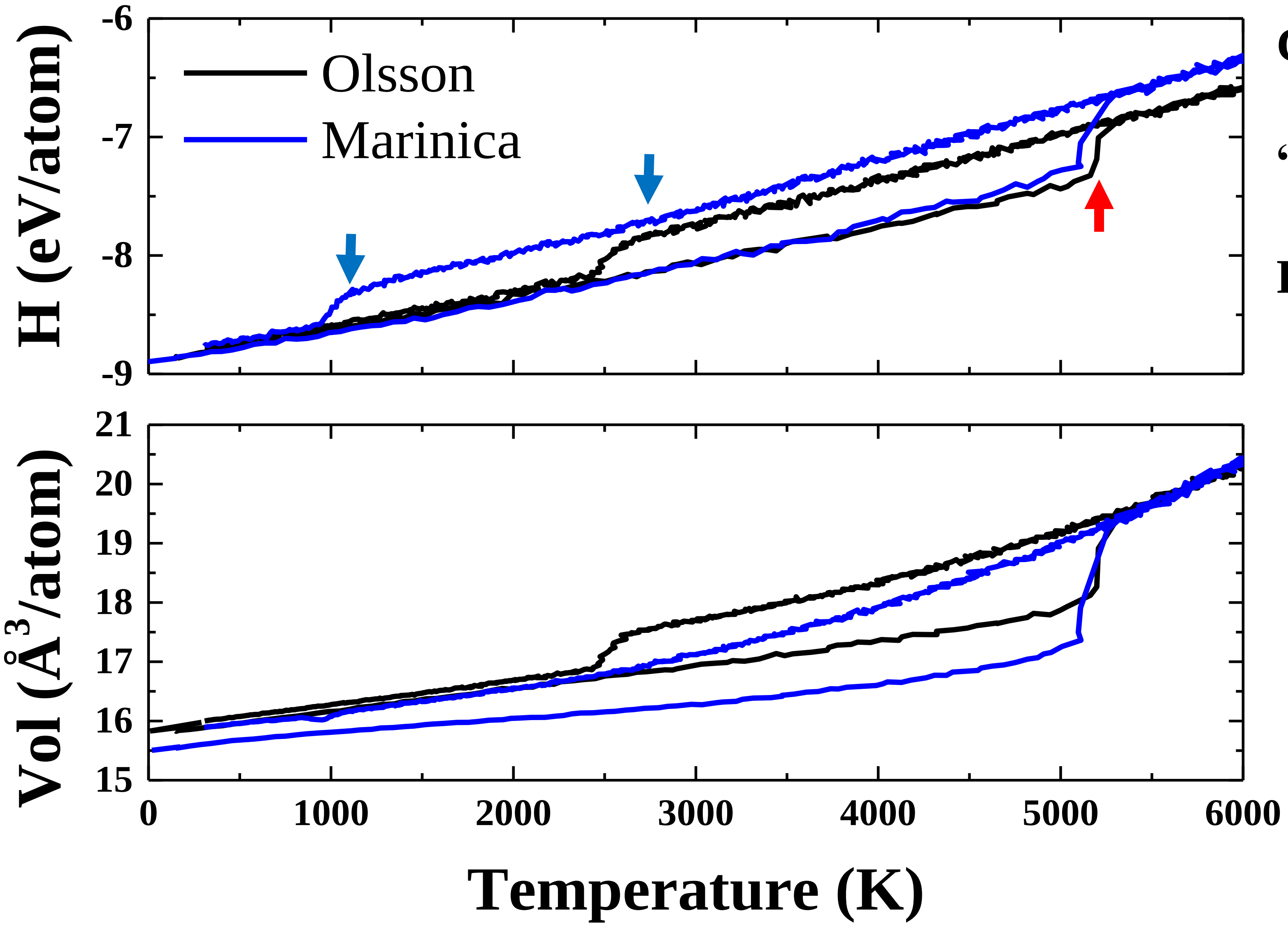


[1] A. Nuttall et al. A thermodynamic analysis of hypervelocity impacts on metals. Int. J. of Impact Eng. 144, (2020)

EOS



[1] Litasov, K. D. et al. Journal of Applied Physics, 113(13), 133505 (2013).



C_p (T) is similar from both FFs

“Melting” ,T+, at same T.

Recrystallization at diff. T.

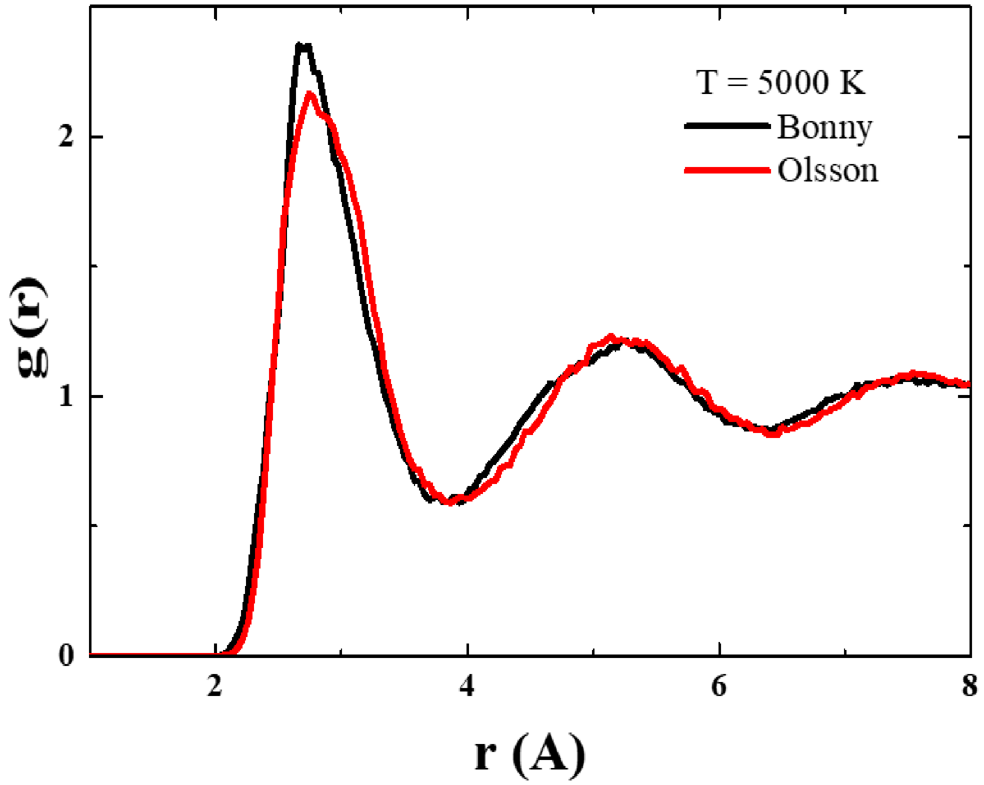
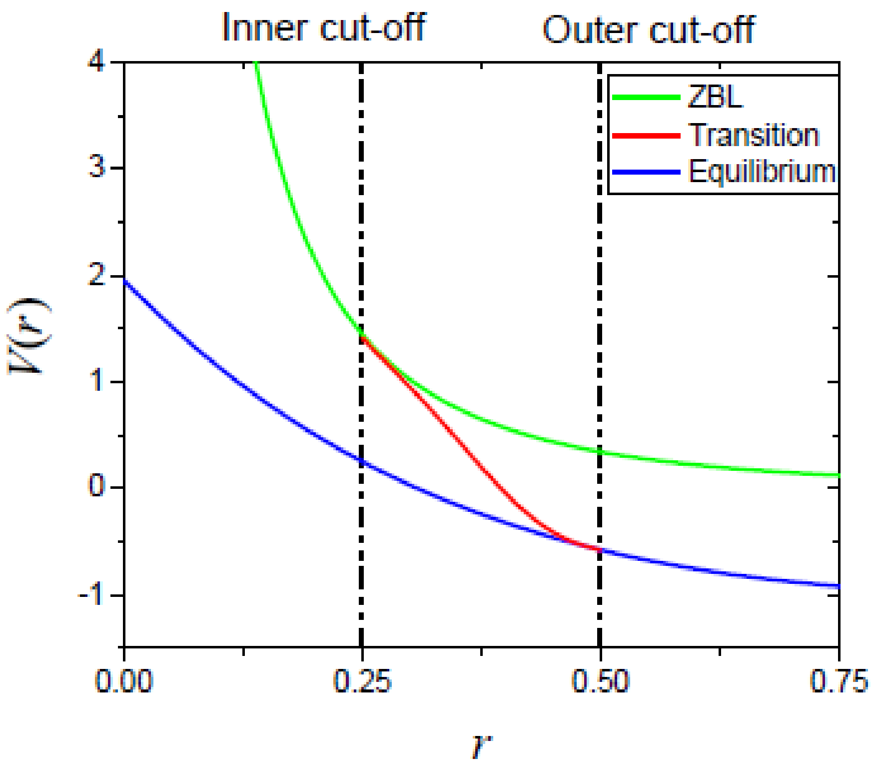
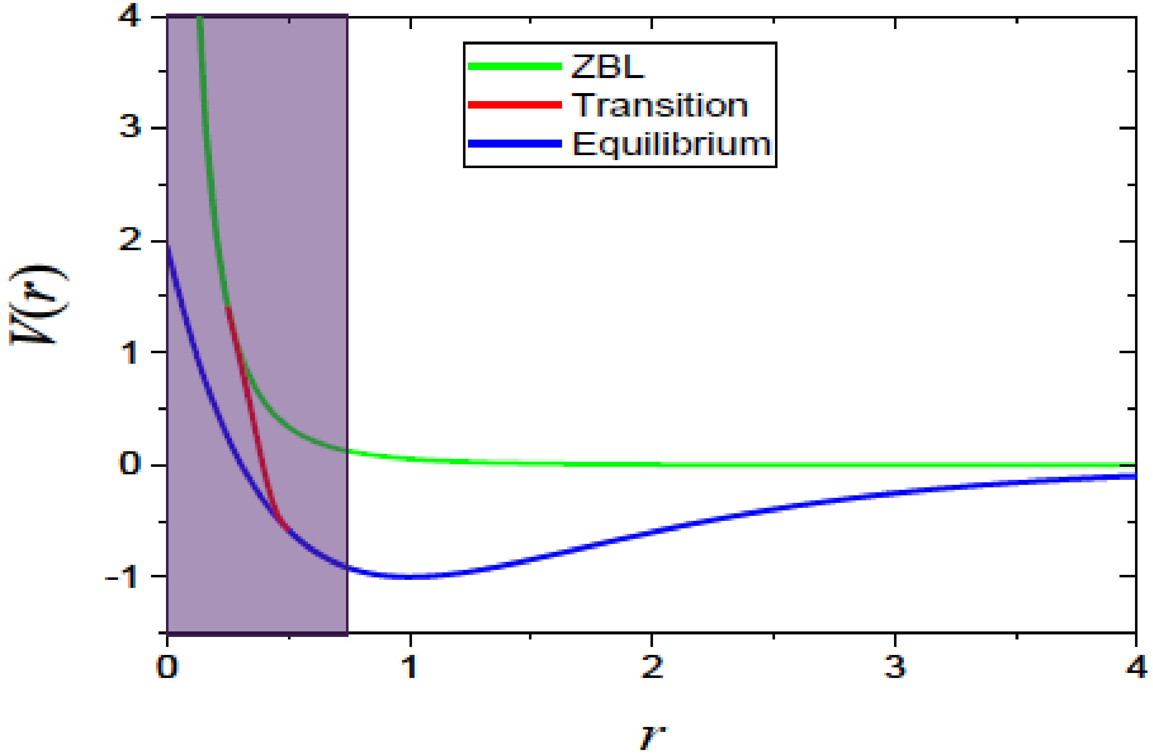


FIG. 1 The RDF for liquid W, T = 5000 K, using two different interatomic potentials.

	Olsson	Marinica	Exp
C_{11}	532	523	523
C_{12}	205	203	203
C_{44}	163	160	160
B (GPa)	313.8	320.0	310.8
T_m (K)	**4102**	**3874**	**3695**
ΔH (kJ/mol)	**40.34**	**48.40**	**52.31**
ΔS (J/molK) as $\Delta H/T_m$	9.83	12.49	9.62
ΔV (cm^3/mol)	8.36	11.1	10.20

A. Fraile et al. Nucl. Fusion 62 (2022), 026034





Stiffened Potentials

$$\boldsymbol{V}(r) = \Theta(r - r_o)\, V_{\text{eq}}(r)$$

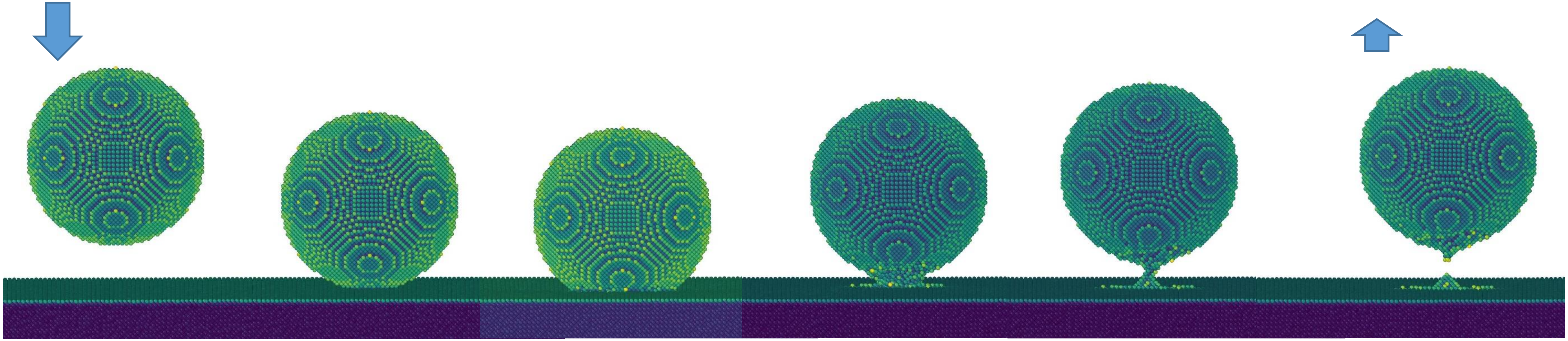
$$+\Theta(r_o - r)\,\Theta(r - r_i)\left\{V_{\text{eq}}(r) + \zeta\left(\frac{r_o + r_i - 2r}{r_o - r_i}\right)\left[V_{\text{nucl}}(r) - V_{\text{eq}}(r)\right]\right\}$$

Smooth transition function

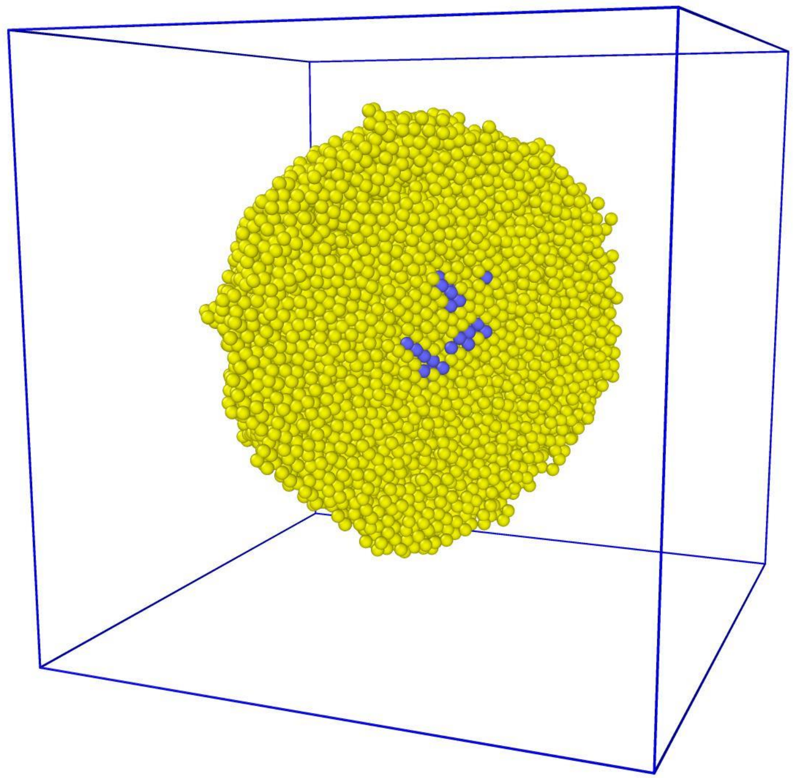
$$+\Theta(r_i - r)\, V_{\text{nucl}}(r),$$

with $\zeta(x) = \frac{3}{16}x^5 - \frac{5}{8}x^3 + \frac{15}{16}x + \frac{1}{2}$

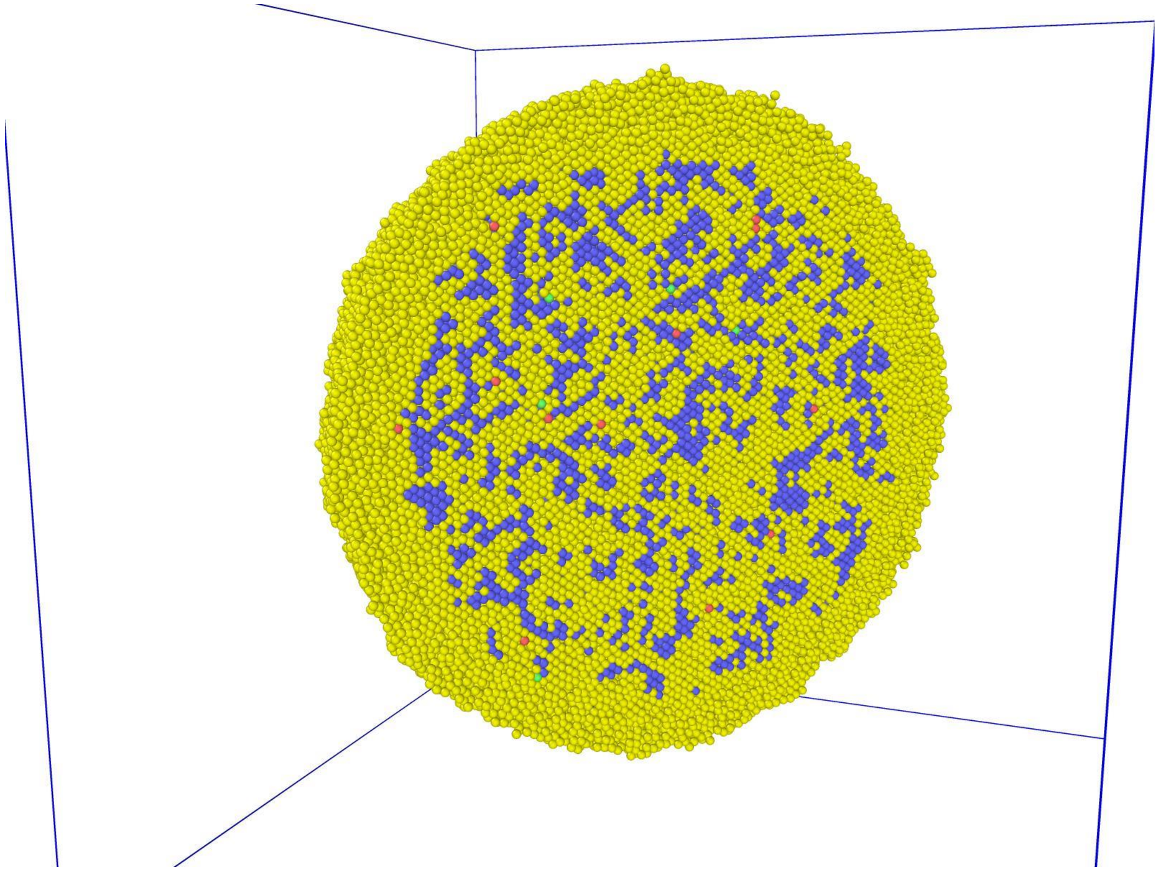
V = 100 m/s



Size-dependent melting point

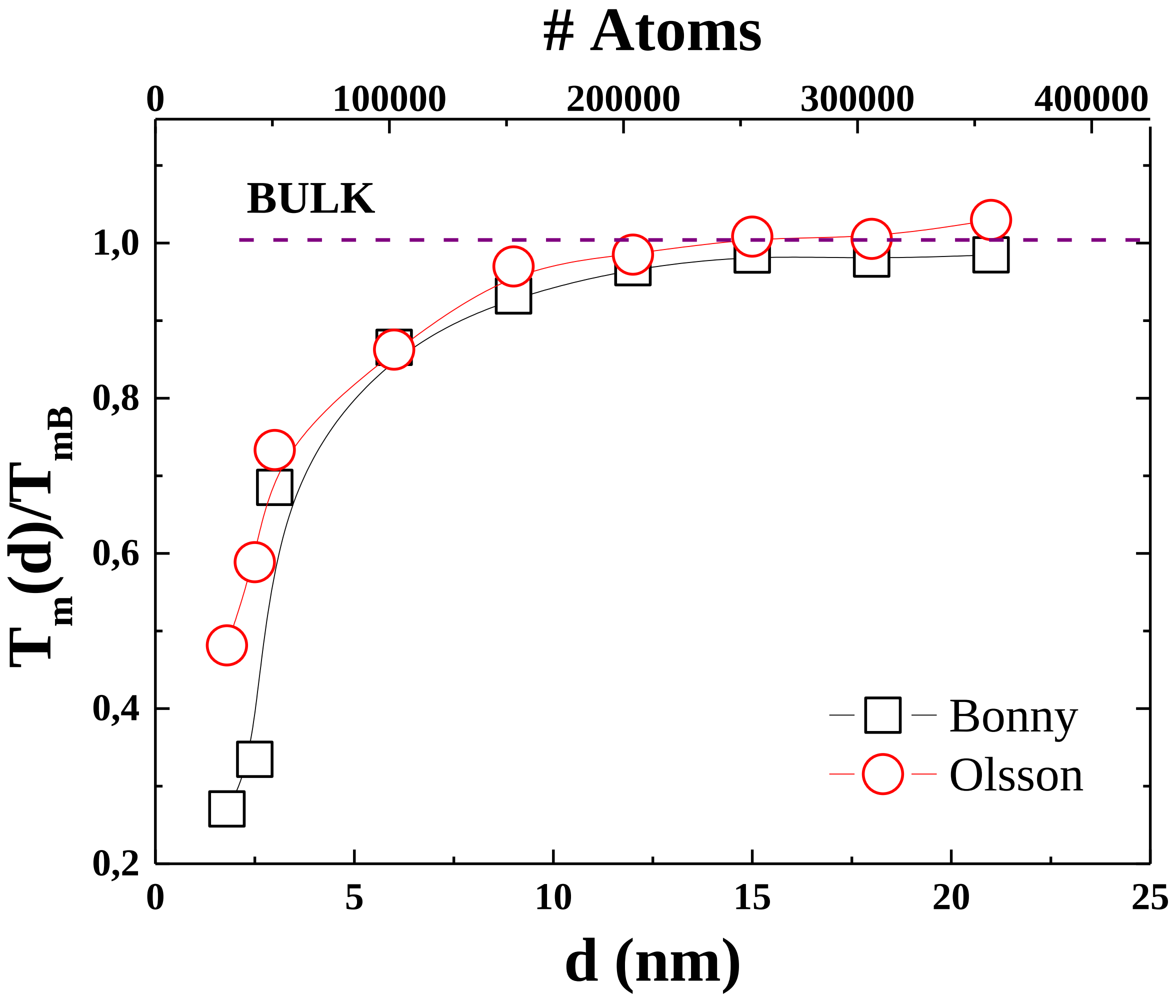


d = 6 nm (8,369 atoms)
$T_m \sim 0.8\ T_{mB}$



d = 21 nm   (359,439 atoms)
$T_m \sim T_{mB}$

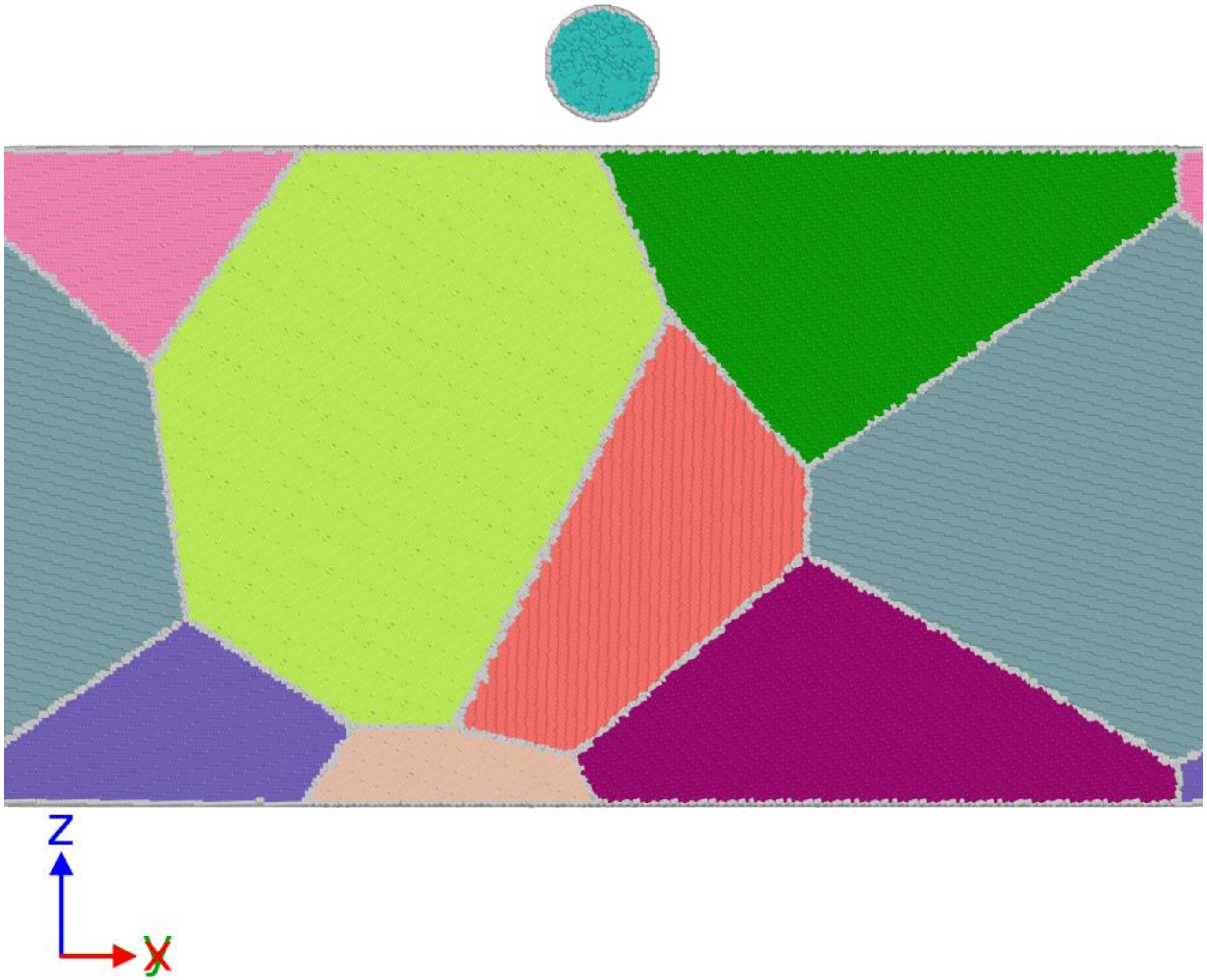
Size-dependent melting point



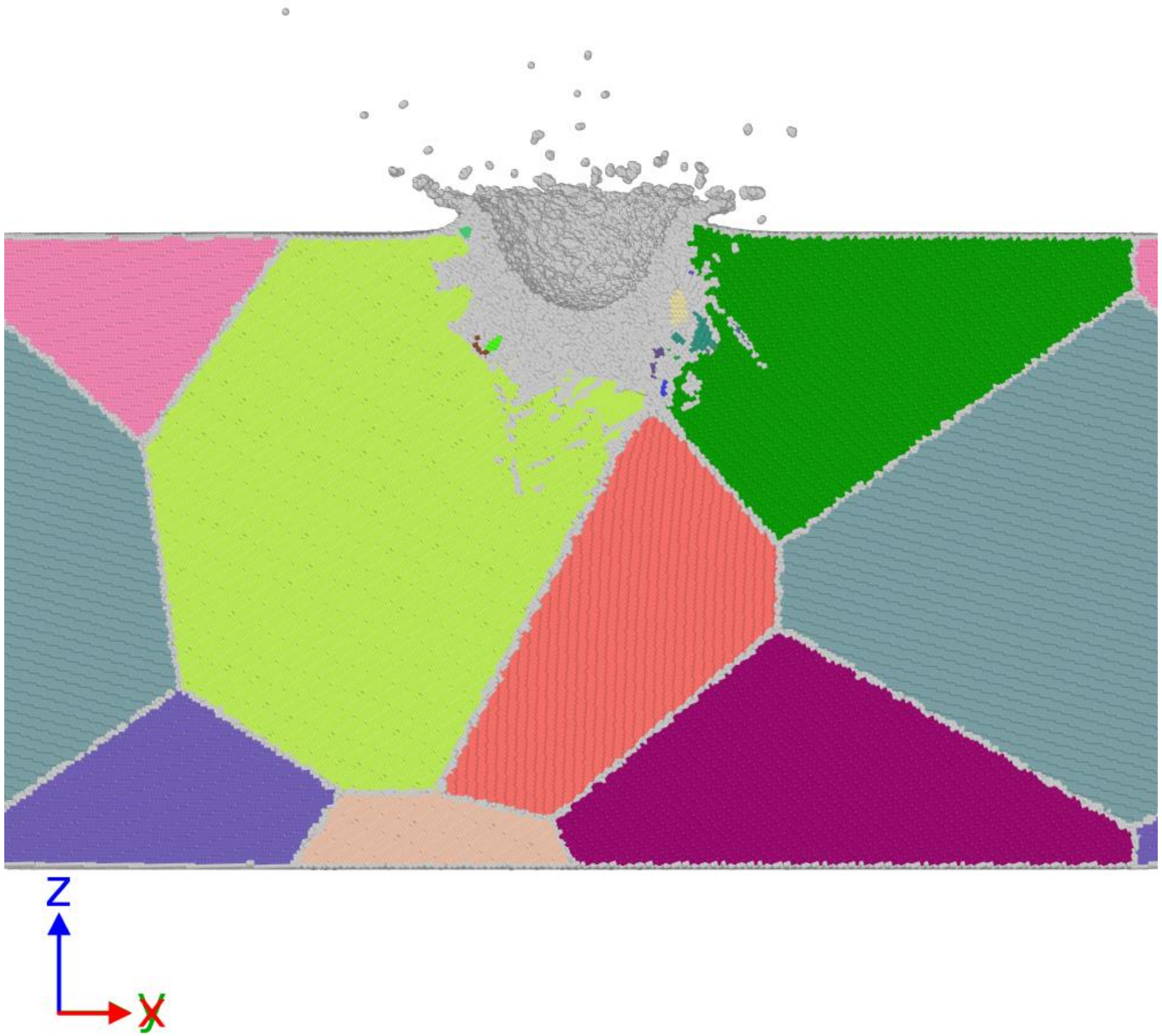
$$T_M(d) = T_{MB}\left(1 - \frac{4\sigma_{sl}}{H_f \rho_s d}\right)$$

T_{MB} = Bulk Melting temperature
σ_{sl} = solid–liquid interface energy
H_f = Bulk heat of fusion
ρ_s = density of solid
d = particle diameter

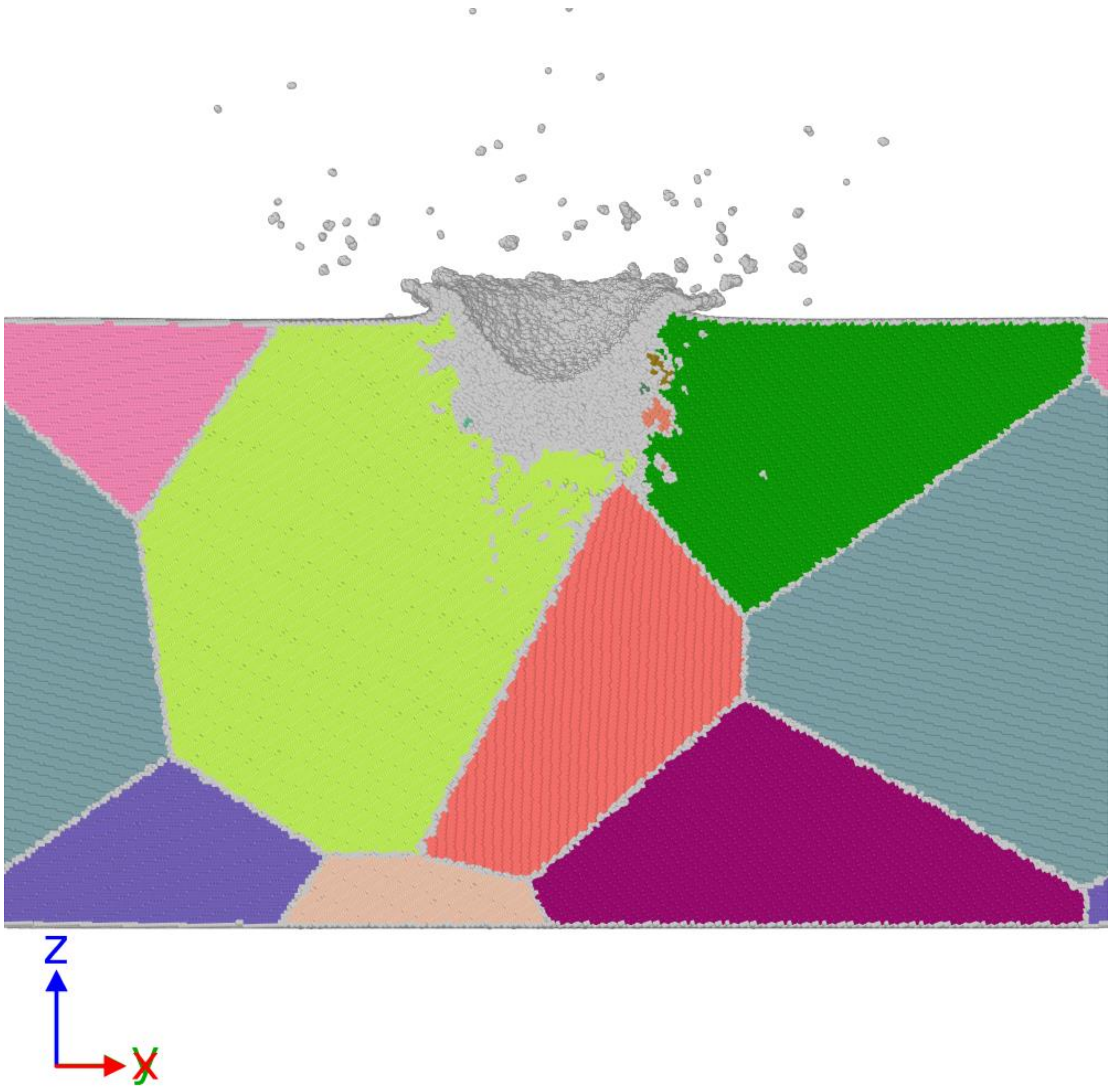
J. Sun & S. L. Simon. The melting behavior of aluminum nanoparticles. Thermochimica Acta. 463 (1–2): 32 (2007)



z
x
y



Z
X



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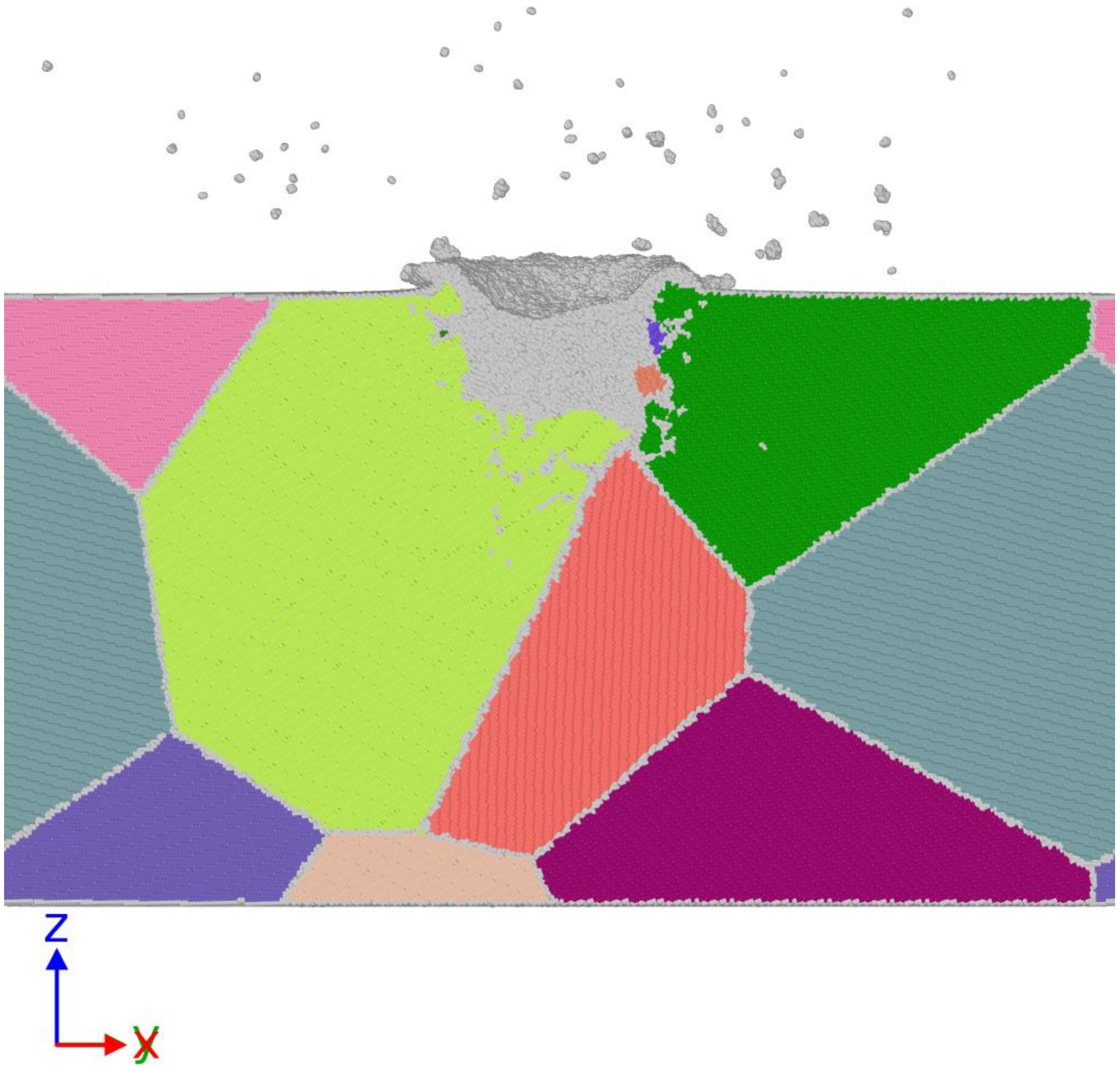
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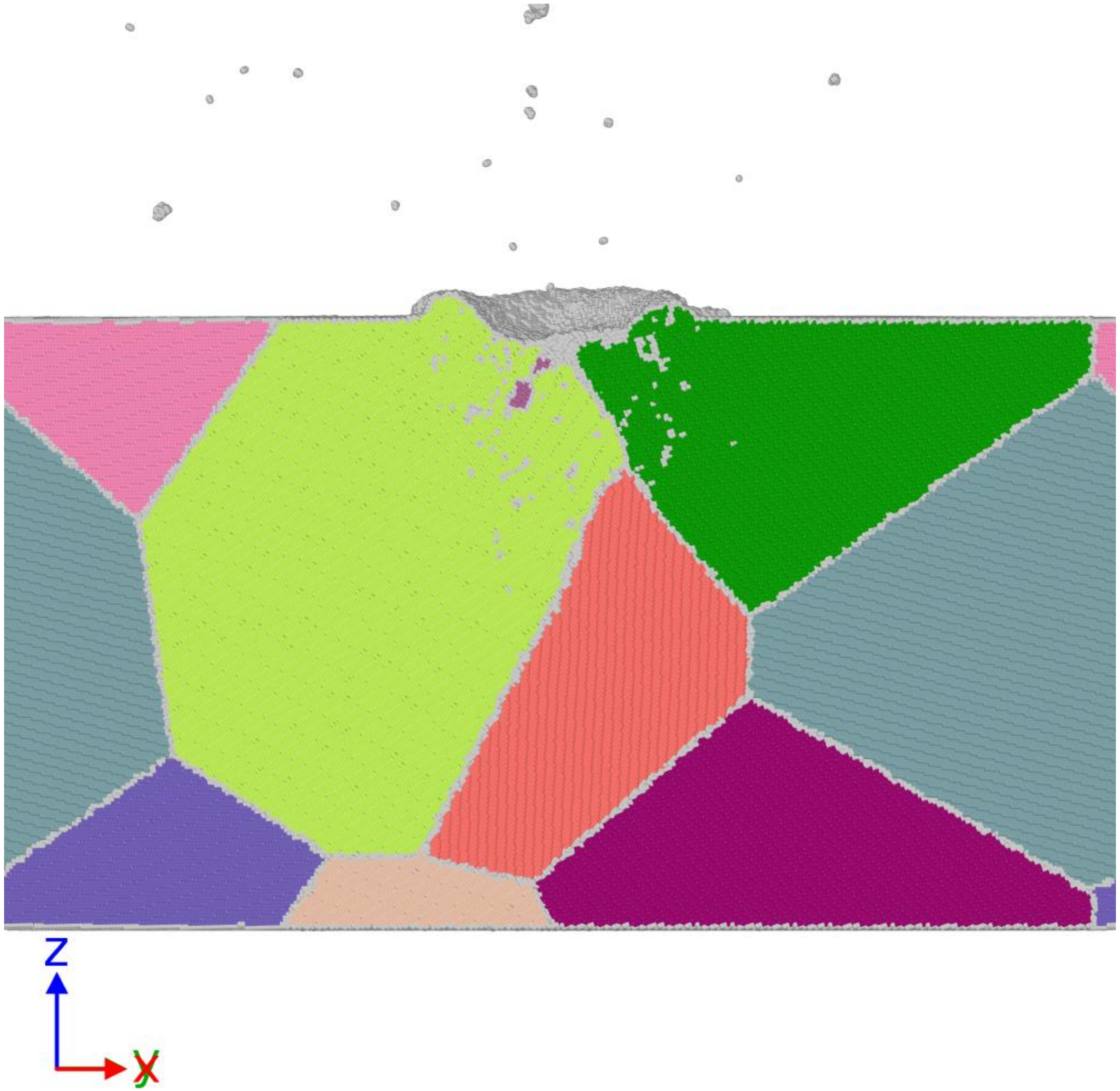
X


Z
X

Magnetism

Laboratory observations of impact-generated magnetic fields

David A. Crawford & Peter H. Schultz

Department of Geological Sciences, Brown University, Providence, Rhode Island 02912, USA

PHYSICAL REVIEW B **103**, 094437 (2021)

Spin-lattice model for cubic crystals

P. Nieves,[1,*] J. Tranchida,[2] S. Arapan,[1] and D. Legut[1]

[1]IT4Innovations, VŠB - Technical University of Ostrava, 17. listopadu 2172/15, 70800 Ostrava-Poruba, Czech Republic

[2]Computational Multiscale Department, Sandia National Laboratories, P.O. Box 5800, MS 1322, Albuquerque, New Mexico 87185, USA

PHYSICAL REVIEW B **105**, 134430 (2022)

Atomistic simulations of magnetoelastic effects on sound velocity

P. Nieves,[1,*] J. Tranchida,[2] S. Nikolov,[3] A. Fraile,[4] and D. Legut[1]

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[2]CEA, DES/IRESNE/DEC, 13018 Saint Paul Lès Durance, France

[3]Computational Multiscale Department, Sandia National Laboratories, P.O. Box 5800, MS 1322, 87185 Albuquerque, New Mexico, USA

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